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Monterey, California

CONTRACTOR REPORT

GAS DYNAMICS OF LASER EXHAUST EXTERNAL TO SPACECRAFT

Shaul Abramovich

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The work reported herein was carried out for the Naval Postgraduate School by Dr. Shaul Abramovich under Contract Number N62271-83-M-1939. The work presented in this report is in support of DARPA project. The work is based on general publications and theory and provides specific means for solving the exhaust flow from a spacecraft laser. Computer programs have been developed to calculate the flowfield in the continuum region as well as in the molecular region. It provides the means to calculate the flux of the exhausted gas towards the walls of the spacecraft. The project on LASER EXHAUST is funded by Defense Advanced Research Projects Agency and is under the cognizance of Distinguished Professor A. E. Fuhs.

This report was prepared by:

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Some procedures have been developed to analyze the flowfield of highly underexpanded axisymmetric ring jets operated at high altitudes. The Method of Characteristics (MOC) was used to compute the Prandtl-Meyer expansion fan and flow parameters in that region. The MOC may also be used to obtain some indications about the repetitive expansion -- compression behavior of the jet as well as the divergent shape of the compression part downstream, when the ambient pressure goes below certain limits.

20. Abstract (continued)

The continuum methods may be used as far as the limit where translational equilibrium ceases to exist. The breakdown of the continuum theory may be evaluated using the experimental breakdown parameter as proposed by G. A. Bird. Beyond this limit, the molecular Direct-Simulation-Monte-Carlo method (DSMC) is applied.

The axisymmetric Monte Carlo Simulation begins outside the nozzle, where the breakdown parameter has a value of approximately 0.05. The actual shape of this breakdown limit is a closed lobe surface which starts at the nozzle lips, approximately follows a specific Mach wave in the Prandtl-Meyer fan and closes back to the axis far downstream. Because our interest is limited to the close vicinity of the corners, there the shape of this limit may be approximated to a straight line (for an axisymmetric flow making a cone).

For the simulation purposes, the domain between the breakdown limit and the wall is divided into sectors, each sector divided into radial regions and each region into simulation cells. Each cell is filled with a number of simulated molecules relative to the cell volume and local number density.

The simulation is performed for each region separately and contains:

* molecular motions
* generation of new molecules to simulate input flows
* deactivation of molecules to simulate output flows
* molecular collisions

Because there is no apriori information about the flow interaction between different regions, the whole simulation is done on an iterative basis. A first run will supply the output flux from each region. These results are used as input data for consecutive runs.

The program runs as far as the collision frequency is still high and the mean free path is low compared with the size of the cells. Beyond this limit the flow may be regarded as collisionless, and the flux towards the solid wall may be computed directly.

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ABSTRACT

Some procedures have been developed to analyze the flowfield of highly underexpanded axisymmetric ring jets operated at high altitudes. The Method of Characteristics (MOC) was used to compute the Prandtl-Meyer expansion fan and the flow parameters in that region. The MOC may also be used to obtain some indications about the repetitive expansion — compression behavior of the jet as well as the divergent shape of the expansion part downstream, when the ambient pressure goes below certain limits.

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I. INTRODUCTION

Gas jets released from spacecrafts and external flows about vehicles at high altitudes have a renewed interest in particular with regard to two main aspects:

a. contamination of the spacecraft walls

b. optical disturbances caused by the plume.

A spacecraft gas dynamics laser releasing a large quantity of gas is highly affected by these two factors and the interest in analyzing them and being able to control them have a unique importance in further development.

A spacecraft laser is assumed to have a long cylindrical shape with the optical power output devices installed at one of its bases as shown in Figure 1.

The output gas is released through a ring nozzle, undergoes a fast three dimensional axisymmetric expansion, and forms a plume covering the whole meridian plane of the vehicle. It widens to large angles of expansion so that it may intersect the laser beam. Back scattered molecules may return to the wall of the spacecraft causing contamination and degradation of surfaces and vehicle parts.

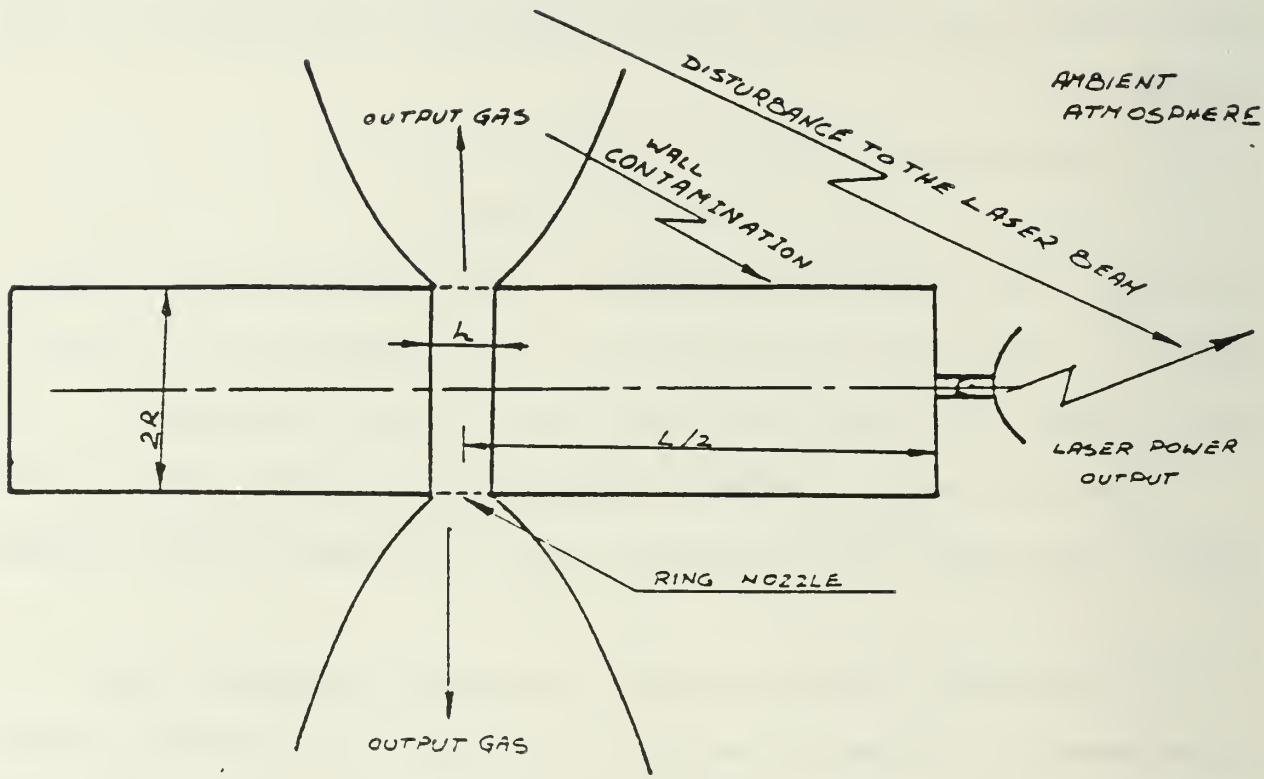


Figure 1. The Spacecraft Laser.

M_o - Mach number at the exit surface ~ 4 the jet gas is composed of two species

heavy molecules $M_{G1} = 19$

light molecules $M_{G2} = 4$

Altitudes between 200 to 1000 km.

Continuum flow theory may be used to solve the flowfield and flow parameters as far as there is translational equilibrium, it means that intermolecular interactions are fast enough to maintain expansion rates. Wherever these interactions are too slow, the continuum flow becomes invalid and the molecular flow theory should be employed.

The solution for the continuum regime is computed here by means of the Method of Characteristics (MOC) [1,2,3]. The limit where continuum breakdown occurs was estimated by the experimental breakdown parameter as proposed by G. A. Bird [4]. Beyond this limit, it is proposed to compute the molecular flow by means of the Direct Simulation Monte Carlo technique as described in detail by Bird [4].

For moderate and low pressure ratios (static pressure at the nozzle exit to the ambient pressure), an underexpanded jet exhibits a repetitive expansion - compression behavior with a geometry depending on the initial Mach angle, on the Prandtl-Meyer fan angle, and on the gas specific heats ratio. For lower ambient pressure which occurs at higher altitudes, the first compression region is pushed out to the envelope of the jet forming the barrel shock. If the ambient pressure is low enough, this compression region may disappear due to the molecular behavior of the flow [6,11].

The breakdown of the continuum theory occurs in a region where the gas density and pressure are high compared with the density and pressure in the ambient gas. At high altitudes the ratios between these parameters may reach 10^6 or more. Considering this range of variations, computational validity dictates the use of the Direct Simulation Monte Carlo method. In the higher density range the jet will be considered as consisting of two species of gas, their molecular model will be "the hard sphere molecule" model and

ambient gas is not allowed to protrude. In the lower density region the flow will be regarded as collisionless.

In the following chapters we bring the detailed description of the computer programs which solve the different parts of the flowfield.

II. THE CONTINUUM REGIME

A. THE TWO DIMENSIONAL ISENTROPIC UNDEREXPANDED JET

The results brought here are based on the supersonic steady isentropic flow theory as described in literature (see for example, Shapiro [1], Liepman and Roshko [2], and Owczarek [3]).

The ranges of paremeters of a jet emerging from a gas dynamics spacecraft laser are:

a. The Mach number at the exit surface $M_o \approx 4$. The static pressure at the exit plane $P_o \approx 136$pa. Ambient pressure (P_{amb}), temperature (T_{amb}) and other thermodynamic properties of ambient gas depend on the altitude as shown in Table 1. The jet gas may consist of DF, HF, Helium and other species. In the programs we limit the compositon to two species: Air and He. (The program allows changes in the composition and types of gas.)

b. The pressure ratio $\frac{P_o}{P_{amb}}$ for the minimum required altitude (200 km) assures that the jet is highly underexpanded (we show later the influence of this ratio on the shape of the jet).

The following thermodynamic relations are valid as long as the compessible flow is isentropic

$$T_T = T(1 + \frac{\gamma-1}{2} M^2) \tag{1}$$

$$P_T = P(1 + \frac{\gamma-1}{2} M^2)^{\frac{\gamma}{\gamma-1}} \tag{2}$$

$$\rho_T = \rho(1 - \frac{\gamma-1}{2} M^2)^{\frac{1}{\gamma-1}} \tag{3}$$

TABLE 1

ATMOSPHERIC DATA
(Abstracted from U.S. Standard Atmosphere 1976)

Altitude km	Pressure m bar	number density m^{-3}	particle speed m/sec	collision frequency sec^{-1}	mean free path m	molecular weight kg/kmol	density kg/m^3	temperature °k
100	3.2011 -4	1.189 +19	381.4	2.68 +3	1.42 -1	28.4	5.604 -7	195.08
200	8.4736 -7	7.182 +15	921.6	3.9	2.4 +2	21.3	2.541 -10	854.56
300	8.7704 -8	6.509 +14	1079.7	4.2 -1	2.6 +3	17.73	1.916 -11	976.01
400	1.4518 -8	1.056 +14	1148.5	7.2 -2	1.6 +4	15.98	2.803 -12	995.83
500	3.0236 -9	2.192 +13	1215.0	1.6 -2	7.7 +4	14.33	5.215 -13	999.24
600	8.2130 -10	5.950 +12	1356.4	4.8 -3	2.8 +5	11.51	1.137 -13	999.85
700	3.1908 -10	2.311 +12	1627.0	2.2 -3	7.3 +5	8.00	3.070 -14	999.97
800	1.7036 -10	1.234 +12	1954.3	1.4 -3	1.4 +6	5.54	1.136 -14	999.99
900	1.0873 -10	7.876 +11	2192.6	1.0 -3	2.1 +6	4.40	5.759 -15	1000.00
1000	7.5138 -11	5.442 +11	2318.1	7.5 -4	3.1 +6	3.94	3.561 -15	1000.00

where T_T, P_T, and ρ_T are the total temperature, pressure and density (constant for isentropic field). T, P, and ρ are local temperature, pressure and density γ is the specific heat ratio of the gas (considered here as constant), M is the local Mach number.

The partial differential equation of motion for supersonic 2-D irrotational and isentropic flow is a hyperbolic equation having solutions obtained from invariants along characteristic lines. Physical interpretation of these lines are the compression or expansion waves which are oriented at Mach angles relative to the streamlines.

Once the directions of the characteristics (waves) are determined everywhere in the field, all other parameters may be calculated.

B. THE TWO DIMENSIONAL PLANAR JET

The compressible supersonic jet flow is characterized by two families of characteristics (pressure waves) starting at each corner of the nozzle lips. Each of these families of waves forms a Prandtl-Meyer fan. The streamlines crossing the characteristic waves bend outwards resulting in an increase in the flow area. The angle μ between the streamline and the pressure wave is a function of the local Mach number as

$$\mu = \arcsin (1/M) \tag{4}$$

The symbol μ is the Mach angle.

Using the isentropic relations, we can find the relation between the turning angle (θ) and the local Mach number (M) as

$$d\theta = - \frac{(M^2 - 1)}{M(1 + \frac{\gamma-1}{2} M^2)} dM \qquad (5)$$

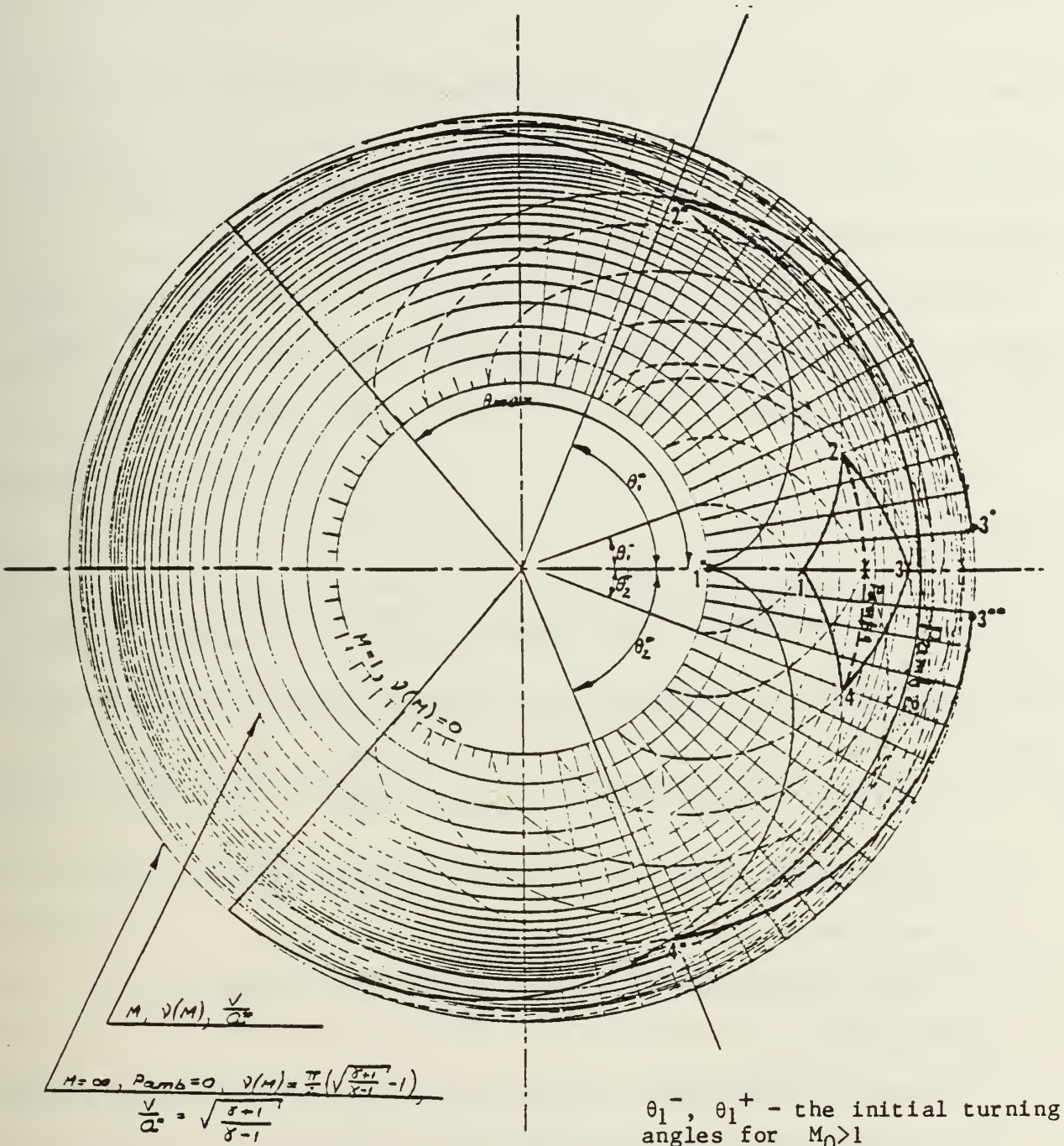
Integration between the conditions M=1 and M gives the total turning angle starting at the throat (where M=1) up to a point with given M. The result gives the Prandtl-Meyer function (angle) as

$$\nu(M) = \frac{\gamma+1}{\gamma-1} \text{ arctg } \frac{\gamma-1}{\gamma+1} (M^2-1) - \text{arctg } (M^2-1) \qquad (6)$$

In the close vicinity of the nozzle lips where the two families of characteristics do not intersect with each other there is a "simple region" of expansion. There the flow parameters are defined by ν and θ of each characteristic line. Further downstream the waves intersect each other. In this part of the flow parameters are defined by the two intersecting characteristics. A singularity occurs when the initial Mach number is unity and a special treatment is required to start the calculations at that point (this special treatment has not been brought here). A particular importance of the Prandtl-Meyer function is when analyzing the two dimensional flow using the hodograph plane.

C. THE HODOGRAPH PLANE FOR A TWO DIMENSIONAL JET

The hodograph plane is a representation of the flow parameters in the velocity plane. Figure 2 shows a hodograph plane calculated for a simple gas (γ=1.4). The circles represent constant Mach numbers and constant



θ_1^-, θ_1^+ - the initial turning angles for $M_0>1$
θ_1^*, θ_2^* - maximum turning angles for a highly under-expanded jet
θ_{max} - maximum turning angle for the specific gas.

Figure 2. The Hodograph Plane.

1-2-3-4-1 defines a jet with $M_0>1$ expanding into $P_{amb1} < P_o$, resulting simple repetitive expansion-compression.
1*-2*-3*-3**-4*-1* defines a jet with $M_0=1$ expanding into $P_{amb2} << P_o$, resulting in a highly underexpanded jet.

pressure ratios $(\frac{P}{P_T})$. The epicycloids are the two families of characteristics. The angles θ are the turning angles due to expansion or compression (which are both present in supersonic jets).

To define an isentropic supersonic jet on the hodograph plane it is necessary to define the Mach number at the exit plane, the pressure ratios $(\frac{P}{P_T})$ and $(\frac{P_{amb}}{P_T})$, and the specific heat ratio (γ) of the gas.

Investigating the shapes of the jet as a function of ranges of parameters we may get:

a. simple underexpanded jets for which $\frac{P_{amb}}{P_T}$ is high enough so that the two families of characteristics intersect each other.

b. a critical underexpanded jet for which $\frac{P_{amb}}{P_T}$ is low enough so that the intersection between the outer characteristic lines of the two familes occur on the outer hodograph circle.

c. highly underexpanded jets for which a part of characteristics do not intersect at all.

d. expansion into complete vacuum so that there are no reflections from the jet boundaries and therefore the compression region disappears.

D. THE SHAPES OF TWO DIMENSIONAL JETS

The following paragraphs further detail the different shapes.

1. Simple Underexpanded Jets

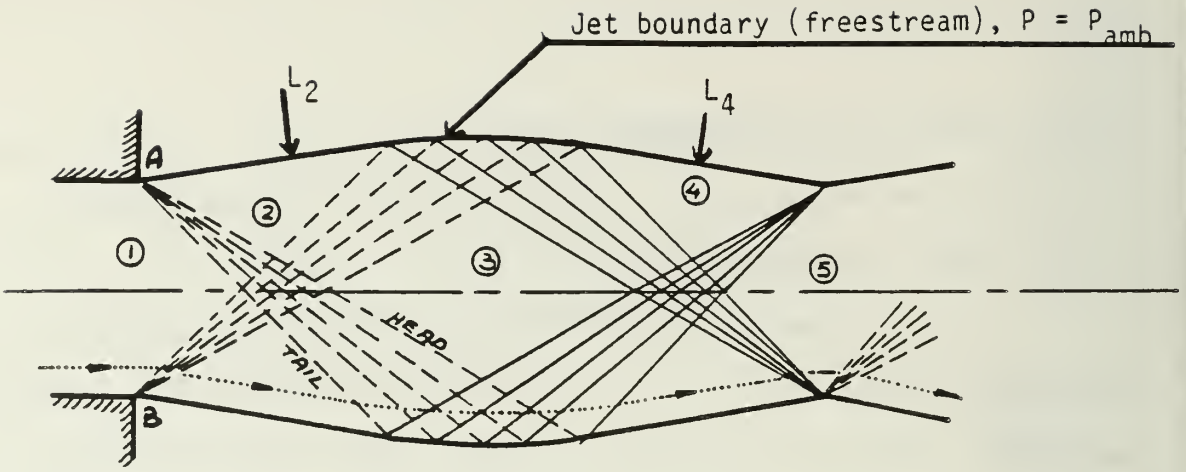
Figure 3 shows the physical plane and the hodograph plane of a simple underexpanded jet. If $M_o>1$, an initial turn of the flow θ_o is made within the nozzle. An aditional turn of θ is due to the underexpansion. θ is found by the intersection of characteristics (1-2) with the circle defined by P_{amb}/P_T .

When $M_o>1$, the characteristic line 1-2 is described in the physical plane by a region in which only one family of expansion waves are present (simple region, see transverse line between 1 to 2 in the physical plane). A different family of expansion waves forms a second simple region when moving between 2 to 3 . At a larger distance from the exit plane, reflected waves from the free streamline (jet boundary) cause compression. An ideal representation of such a jet is a repetitive pattern of expansion and compression.

For $M_o=1$, the tail waves of both families are perpendicular to the flow, thus, both lie on line AB . That means that if $M_o=1$ there is no simple region near the exit plane of the jet. The characteristic line 1-2 on the hodograph plane becomes a single point A (or B) when located in the physical plane.

2. Critical Underexpanded Jets

We define a critical underexpanded jet when point (3) (see Figure 4) lies on the limiting circle M_∞ or $P/P_\infty=0$. This means that there is a core within the jet where the pressure approaches zero and Mach approaches infinity. This core is theoretically bounded at its upstream side by expansion waves and downstream by compression waves.



compression waves

expansion waves

streamline

① uniform axial flow ($P=P_o$)

② uniform flow parallel to L_2 ($P=P_{amb}$)

③ uniform axial flow (lowest pressure-P_{min})

④ uniform flow parallel to L_4 ($P=P_{amb}$)

⑤ uniform axial flow ($P=P_o$)

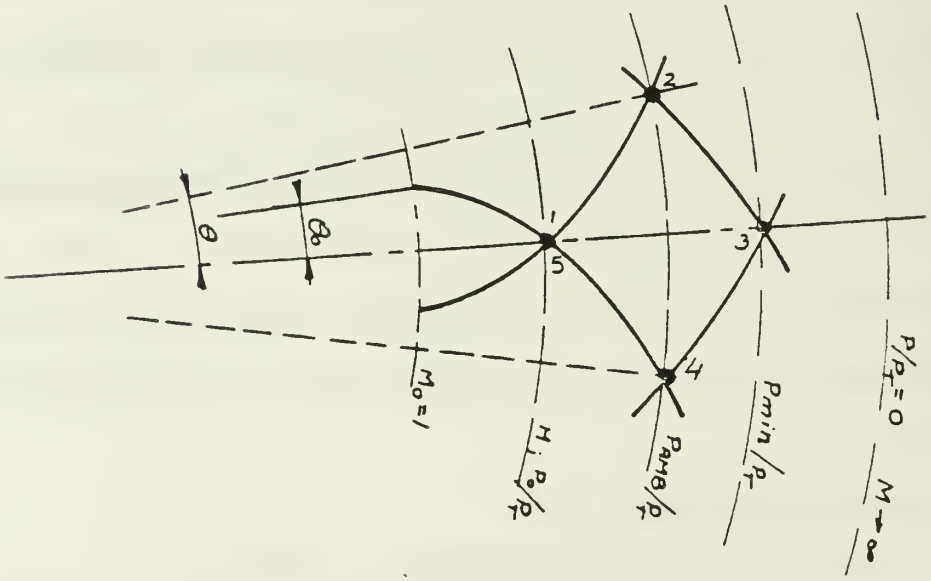


Figure 3. Flow at exit of a simple underexpanded jet.

(a) physical Plane

(b) Hodograph Plane

Using the theoretical expressions for isentropic ideal flow one may derive the values of $\frac{P_{amb}}{P_T}$ or $\frac{P_{amb}}{P_o}$ as function of M_o which causes a jet to be critical underexpanded.

Figure 5 shows results of $\frac{P_{amb}}{P_o}$ as functions of M_o for gases with different specific heat ratio.

3. Highly Underexpanded Jets

When P_{amb} is lower than the critical values as shown in figure 4, point 3 does not exist (there is no intersection between lines 2-3 2'-3'). This means that the repetitive reversible expansion/compression shapes ceases to exist. The envelope of the jet starts at an angle defined by θ at the nozzle exit plane and approaches an asymptotic angle defined by θ_{lim} (see Figure 6).

In this case we get two (symmetric) groups of characteristics C_1-C_2 and C'_1-C'_2 (Figure 6) with no intersection between them. C_1 and C_1' define the inner limit for reflected characteristics, C_2 and C_2' define the outer limit. As the rest of reflected waves lie between C_2 or C'_2 and the jet boundary, we may conclude that a compression region may exist only in a layer along the jet boundary.

Because of irreversible effects such as shear stresses, heat transfer due to high temperature gradients, or condensation effects in real gases, the compression layer may be interpreted as the "barrel shock".

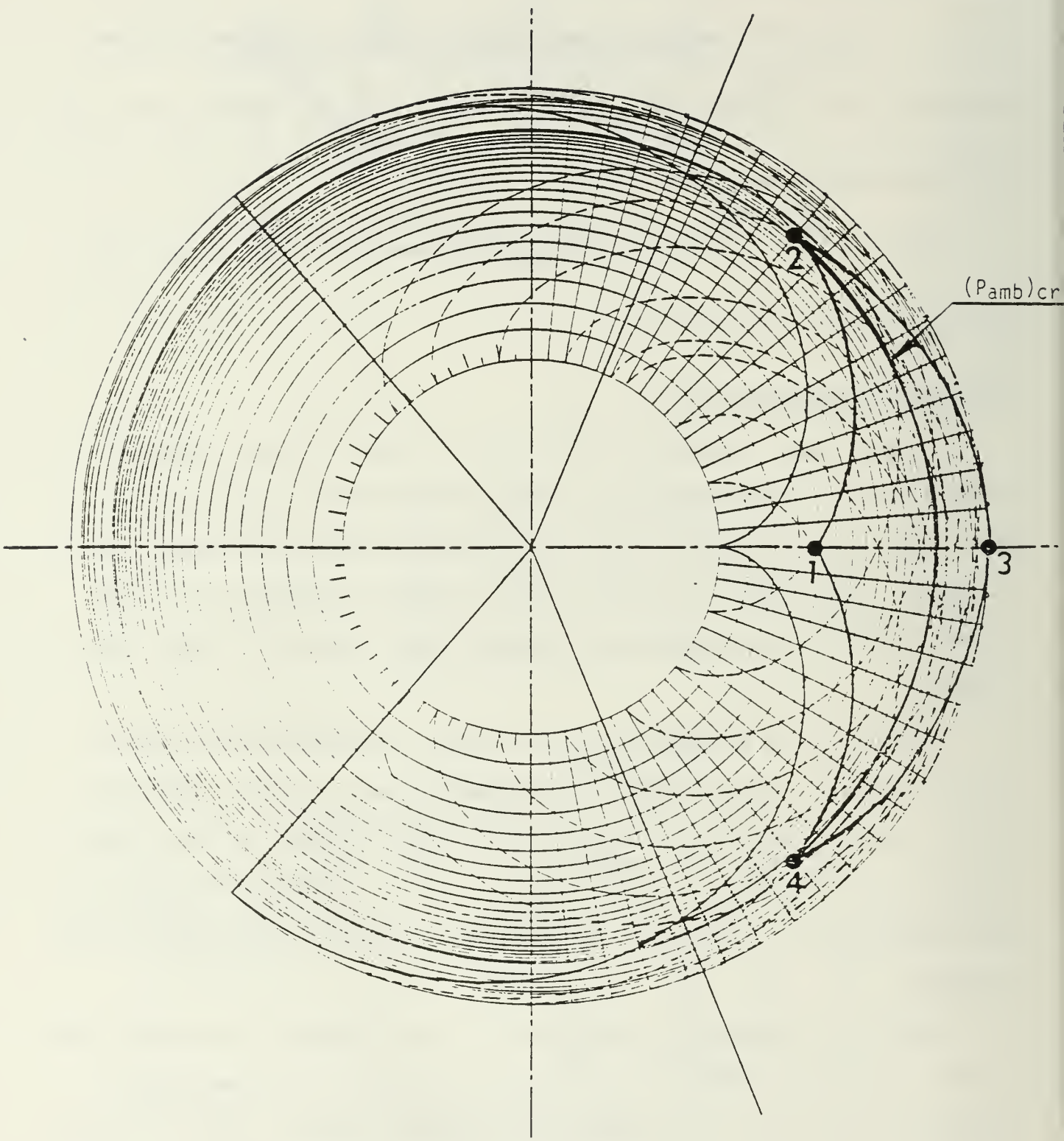


Figure 4. The Hodograph Plane for a Critical Underexpanded Jet. (1-2-3-4-1), (γ=1.4)

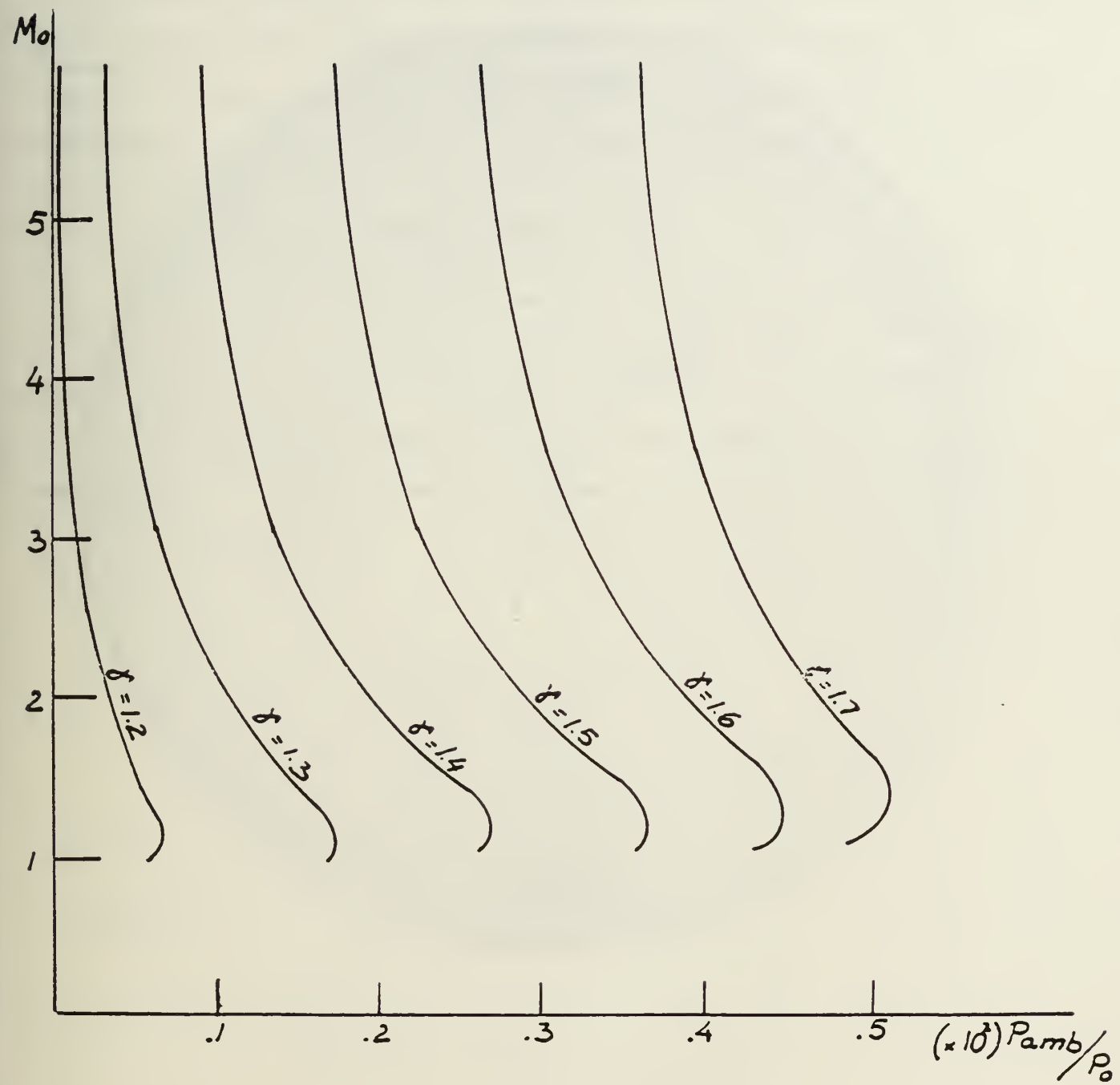


Figure 5. Dependence of critical values of P_{amb}/P_o on the Mach number at the exit plane (M_o) for different values of specific heat ratio (γ).

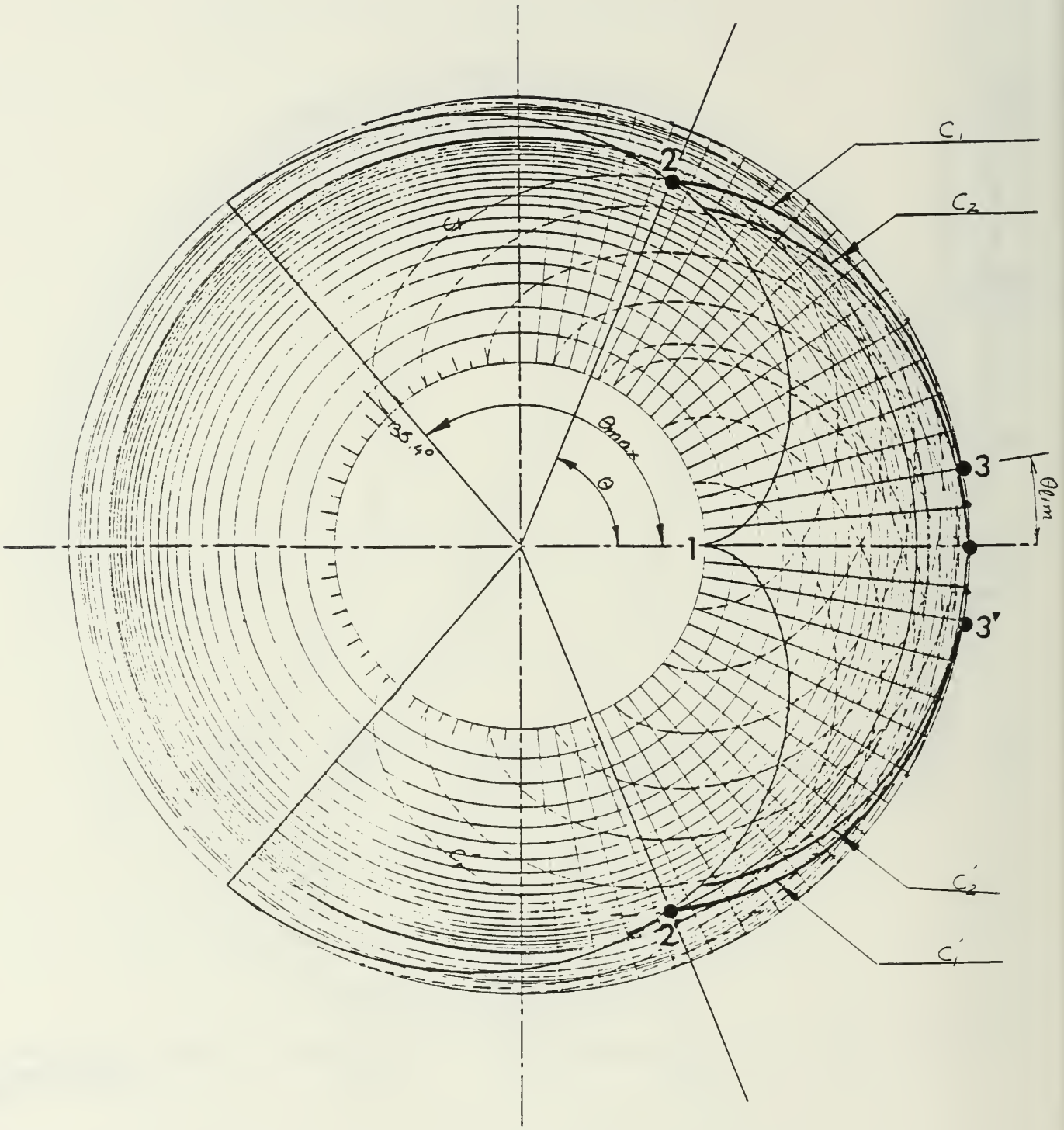


Figure 6. The Hodograph Plane for a Highly Underexpanded Jet

(γ = 1.4)
θ_{max} - maximum turning angle
θ - total turning angle in the specific jet $\theta > \theta_{max}/2$
θ_{lim} - limiting angle of compression region.

Figure (7) shows the hodograph plane for an air jet (γ=1.4) expanding into an ambient pressure 105 times lower than the static pressure at the exit plane. Figure (8) is a schematic description of the jet (the data for this jet is given in Table 2). The shape shown in Figure (8) may be compared with the barrel shock photograph in page 208 Reference [3].

4. EXPANSION INTO A COMPLETE VACUUM - $P_{amb}=0$

This is an extreme situation in which the maximum turn angle of streamlines occur near the nozzle exit plane. The theoretical free stream is defined only by the theoretical turning angles. All streamlines in the flow expanded monotonically towards $P\approx 0$ without being reflected by the jet boundaries.

TABLE 2

CALCULATION OF CHARACTERISTICS ON PHYSICAL PLANE

State	θ_*^+	θ_*^-	θ	$\nu(M)$	M	μ	$\theta+\mu$	$\theta-\mu$	P/P_t
1	0	0	0	0	1	90°	90°	-90°	0.5283
2	0	10	10	10	1.435	44.15	54.15	-34.15	
3	0	20	20	20	1.775	34.3	54.3	-14.3	.2990
4	0	40	30	30	2.135	27.93	57.93	2.07	.1810
5	0	60	40	40	2.54	23.18	63.18	16.82	.1035
6	0	80	50	50	3.013	19.38	69.38	30.62	.55 -1
7	0	100	60	60	3.595	16.15	76.15	43.85	.2672 -1
8	0	120	67.7	67.7	4.145	13.96	88.7	53.74	.1146 -1
9	20	135.4	0	20	1.775	34.3	34.3	-34.3	.5437 -2
10	20	20	10	30	2.135	27.93	37.93	-17.93	.1810
11	20	40	20	40	2.54	23.18	43.18	- 3.18	.135
12	20	60	30	50	3.013	19.38	49.38	10.62	.55 -1
13	20	80	40	60	3.595	16.15	56.15	23.85	.2672 -1
14	20	100	50	70	4.339	13.315	63.32	36.69	.1146 -1
15	20	120	57.7	77.7	5.085	11.34	69.04	46.4	.425 -2
16	40	135.4	0	40	2.54	23.18	23.18	-23.18	
17	40	40	10	50	3.013	19.38	29.38	- 9.38	.55 -1
18	40	60	20	60	3.595	16.15	36.15	3.85	.2672 -1
19	40	80	30	70	4.339	13.315	43.32	16.69	.1146 -1
20	40	120	40	80	5.3479	10.777	50.78	29.23	.4215 -2
21	40	135.4°	47.7	87.7	6.433	8.943	56.64	38.76	
22	60	60	0	60	3.595	16.15	16.15	-16.15	.1146 -1
23	60	80	10	70	4.339	13.315	23.32	- 3.32	.4215 -2
24	60	100	20	80	5.3479	10.777	30.78	9.22	
25	60	120	30	90	6.8190	8.433	38.43	21.57	
26	60	135.4°	37.7	97.7	9.2105	6.2330	43.93	31.5	
27	80	80	0	80	5.3479	10.777	10.777	-10.77	
28	80	100	10	90	6.8190	8.433	18.433	1.57	
29	80	120	20	100	9.2105	6.233	26.23	13.8	
30	80	135.4	27.7	107.7	12.45	4.61	32.3	23.1	
31	100	100	0	100	9.2105	6.233	+ 6.233	- 6.233	
32	100	120	10	110	13.874	4.1331	14.13	5.9	
33	100	135.4	17.7	117.7	21.4	2.678	20.37	15.0	
34	120	120	0	120	27.335	2 097	2.097	- 2.097	
35	120	135.4	7.7	127.7	104	0.546	8.2	7.2	
36	-	-	11°	-	∞	0	-	-	0
51	20	115.4	47.7	67.7°	4.145	13.96		33.7	.5437 -2
52	40	115.4	37.7	77.7	5.085	11.34		26.36	
53	40	95.4	+27.7	67.7°	4.145	13.96		13.7	.5437 -2
54	60	75.4	+ 7.7	67.7°	4.145	13.96		- 6.26	.5437 -2
55	60	95.4	17.7	77.7	5.085	11.34		6.4	
56	60	115.4	27.7	87.7	6.433	8.943		18.8	

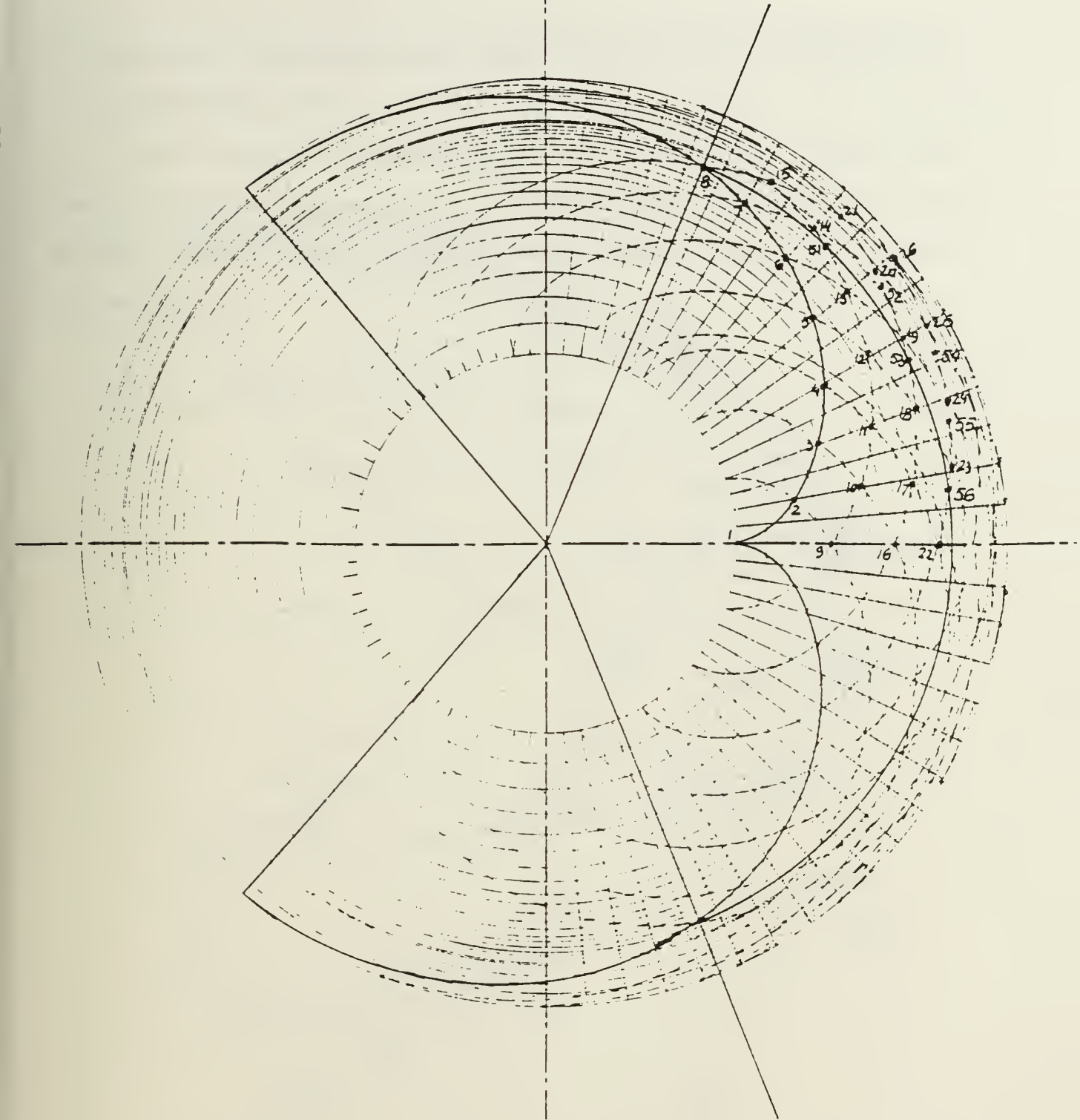


Figure 7. Hodograph plane showing the points on the mesh of characteristics. (Related to physical plan Figure 8).

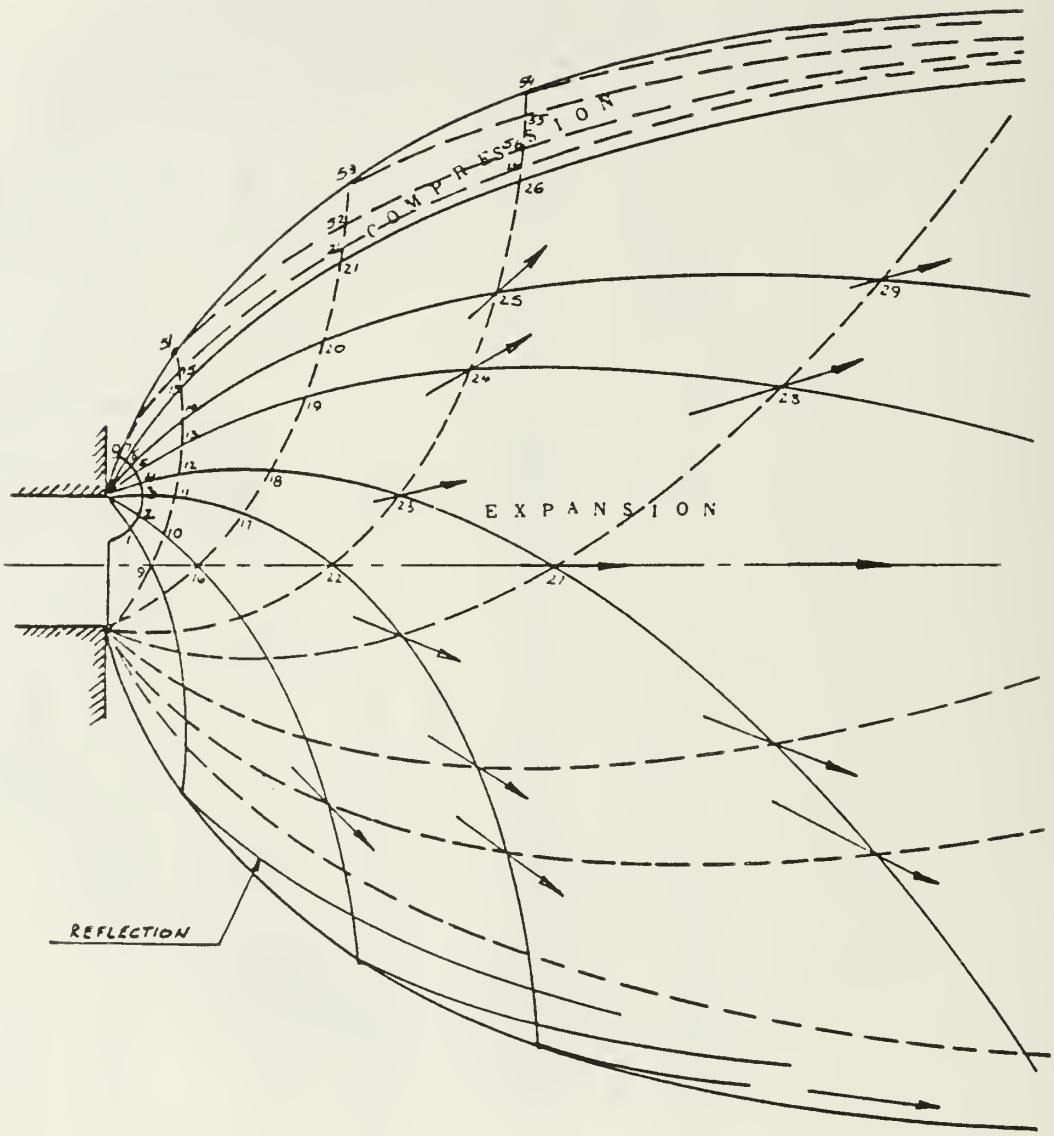


Figure 8. Schematic shape of a highly underexpanded jet.

(See Figure 7 - The Hodograph Plane)

The arrows indicate flow direction.

E. THE METHOD OF CHARACTERISTICS; COMPUTATION OF PLANAR AND AXISYMMETRIC TWO-DIMENSIONAL FLOWS

For a planar two dimensional flow, the Prandtl-Meyer function ν and flow direction θ at any point (3) in the field may be calculated using data of two other points (1) and (2) located on characteristic lines that intersect at (3) (see Fig. (9))

$$\nu_3 = \frac{1}{2}(\nu_1 + \nu_2) + \frac{1}{2}(\theta_1 - \theta_2) \tag{7}$$

$$\theta_3 = \frac{1}{2}(\nu_1 - \nu_2) + \frac{1}{2}(\theta_1 + \theta_2) \tag{8}$$

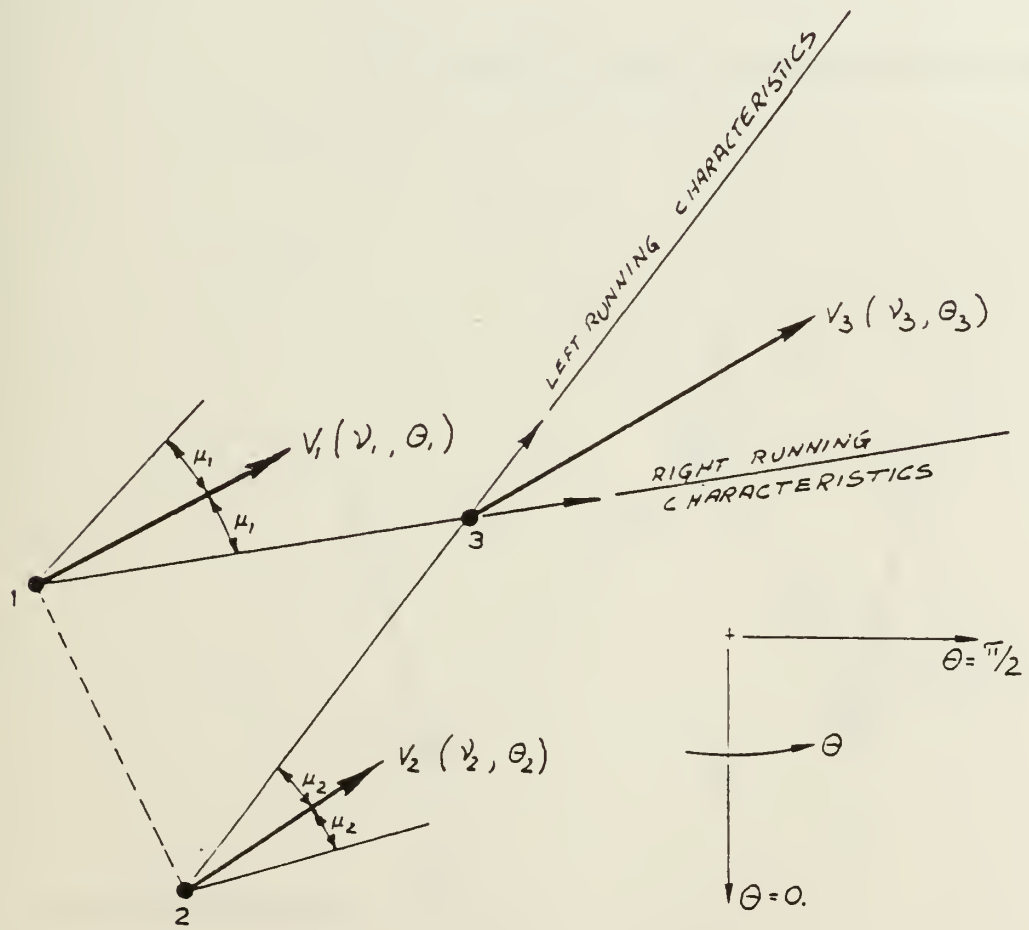


Figure 9. The calculation of ν and θ for point (3) is based on data for points 1 and 2.

For axisymmetric, two-dimensional flow, Liepmann and Roshko [2] developed expressions for finding the Prandtl-Meyer function (ν) and the flow direction (θ) which are given by:

$$\nu_3 = \frac{1}{2}(\nu_1 + \nu_2) + \frac{1}{2}(\theta_1 - \theta_2) + \frac{1}{2}\left[\sin \mu_1 \frac{\sin\theta_1}{r_1} \Delta\xi_{13} + \sin \mu_2 \frac{\sin\theta_2}{r_2} \Delta\eta_{23}\right] \tag{9}$$

$$\theta_3 = \frac{1}{2}(\nu_1 - \nu_2) + \frac{1}{2}(\theta_1 + \theta_2) + \frac{1}{2}\left[\sin \mu_1 \frac{\sin\theta_1}{r_1} \Delta\xi_{13} - \sin \mu_2 \frac{\sin\theta_2}{r_2} \Delta\eta_{23}\right] \tag{10}$$

The angles and subscripts are shown in Figure (10).

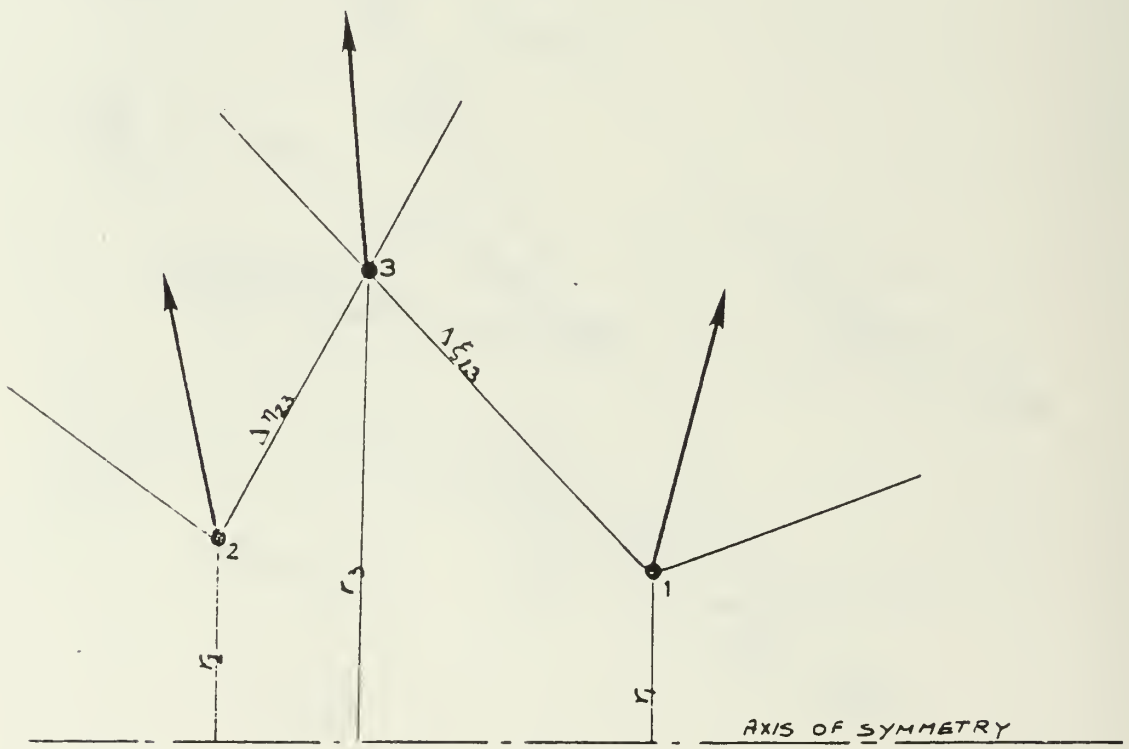


Figure 10. Calculation of θ and ν for axisymmetric flow.

It is obvious that for the axially symmetric flows the increase in the radius causes the increase in the flow cross section and influences the flow direction and the Prandtl-Meyer function. These facts have been taken into account when developing the "compatibility equations" (9,10).

Using equations (9,10) we have developed a computer program which enables the calculation of the jet flow for a two dimensional and for an axially symmetric geometry (ring jet).

The listing of the program, the program description and some results are given in Appendix A.

III. THE BREAKDOWN OF THE CONTINUUM THEORY

A. GENERAL CRITERIA

As described in detail by Bird (Chapter 1 Reference [4]), the validity of the continuum approach has been identified with the validity of the Navier Stokes equations. This requires that the Knudsen number $K_n = \lambda/L$ should be small compared with unity (λ is the mean free path and L is a scale length for the specific flow field). For K_n larger than a certain limit (between 0.01 to 0.1 depending on the required accuracy) a microscopic approach is necessary.

For small values of L , the microscopic approach may lead to statistical fluctuations of the results due to the small number of molecules participating in the flow processes. In figure (11) which was reproduced from Bird's book [4, figure 1.6], the regimes of rarefied flow and high fluctuations are depicted. The flow around the jet-air boundaries near a spacecraft is generally rarefied (high Knudsen number), but has insignificant fluctuations.

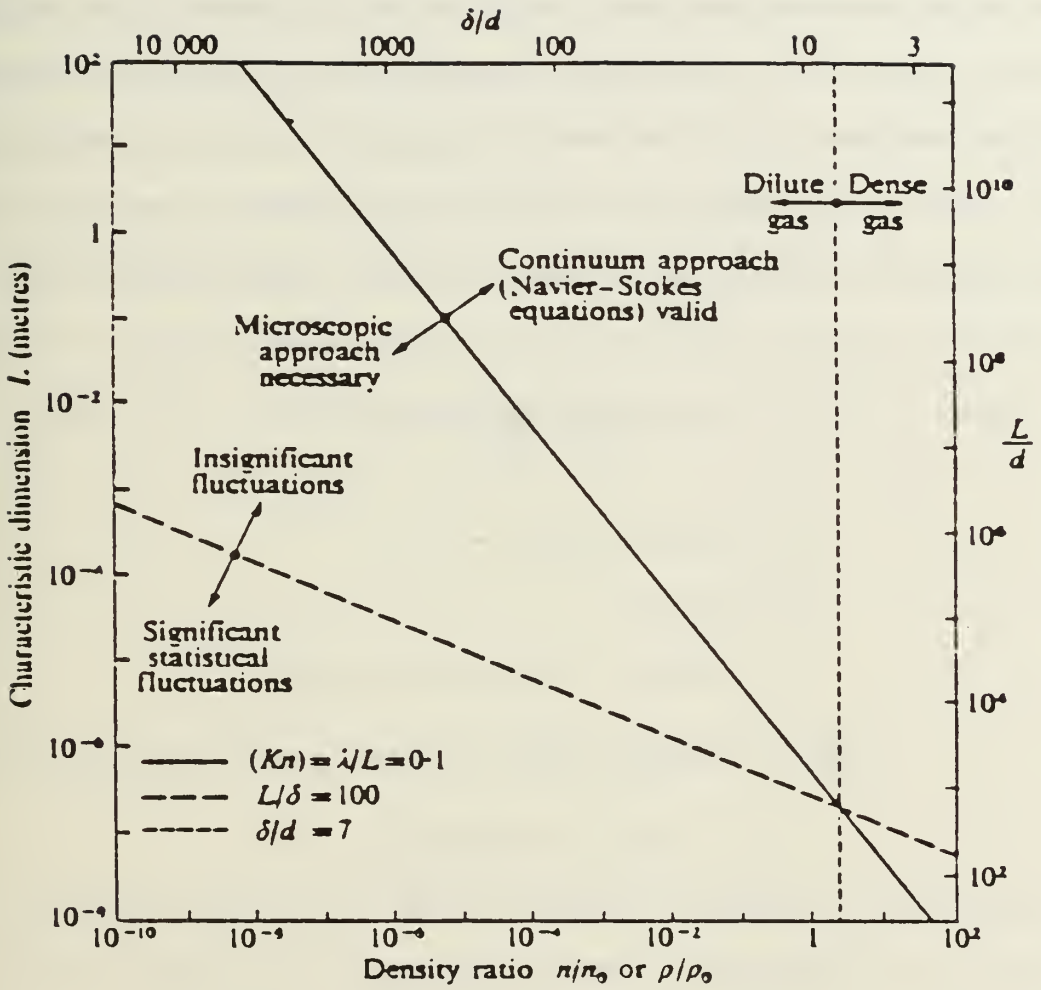


Figure 11. Limits for continuum approach and microscopic approach ($d=3.7 \times 10^{-10}$ m).

B. THE EMPIRICAL CRITERION

The Method of Characteristics (MOC) was used to compute the jet flow and the results obtained from the computer program "AXSYM" are valid as long as the continuum flow theory is valid.

The continuum flow requires that the mean free path should be negligibly small in comparison with the scale length of the macroscopic flow variations. The classical theory for Prandtl-Meyer expansion may therefore be expected to fail at progressively larger distances from the nozzle lips as the gas density decreases with the increasing flow angle and Mach number. The empirical criterion for the breakdown of continuum flow in steady expansion flow [4] is that

$$P \equiv \frac{q}{\rho \nu} \left|\frac{d\rho}{dS}\right| \simeq 0.05 \qquad (11)$$

where q = stream velocity

ρ = density

ν = molecular collision frequency

$\left|\frac{d\rho}{dS}\right|$ = absolute change in density while moving a distance dS along a streamline

Introducing the breakdown parameter P into the program, gives the definition of the boundary where the flow should be calculated by means of the molecular flow theory, i.e., by solving the Boltzmann equation.

For an underexpanded jet with a high initial Mach number, the breakdown surface is nearly a streamline. Furthermore, the range of flow parameters for the present problem are such that the simple region extends to very large distances and near the nozzle lip the breakdown limit may be approximated by a straight line.

For the axisymmetric jet there is no simple region, however, for the region of interest it may be regarded as linear.

The method proposed in the present work for solving the flow behind the breakdown boundary is the Direct Simulation Monte Carlo (DSMC). For this purpose, a computer program "SIMUL" was developed. In the following chapter we describe the algorithms required for the specific problem, the geometry and the data organization. Detailed program description is given in Appendix (B).

IV. THE MOLECULAR FLOW IN AN AXISYMMETRIC RING JET

A. GENERAL CONSIDERATIONS

The part of the field in which the jet may be calculated by means of the continuum theory was described in Chapter II. There we calculated also the boundaries where continuum theory becomes invalid and molecular calculation should be employed. In fact, the molecular theory and the molecular Boltzmann equations are universal and hold for the entire flowfield. However, computational requirements make the Boltzmann equation impractical for the upstream flows. Therefore we limit our solution only to the part of the flow beyond the region where continuum breakdown occurs.

As a result obtained from MOC solution the "breakdown", i.e., the locus where the breakdown parameter p has values between 0.03 to 0.06, for the region close to the nozzle lips this boundary may be approximated by a straight line (for axisymmetric flow this line is the envelope of a cone, see Figure (12)).

For the specific jet and gas, the breakdown occurs in a region where the number density is in a range of 10^{21} molecules/m^3. For ambient gas at an altitude of 200 km the number density is 10^{15} and decreases to a range of 10^{11} at 1000 km. In order to be able to express this vast change in a simulation, we would need to have an extremely large number of cells which would be impossible to store in a computer. To overcome this problem we are required to make a less exact formulation which enables the production of results, having to pay the penalty of "smearing" the steep gradients and obtaining averages within layers of simulated cells. Unfortunately it is impossible to

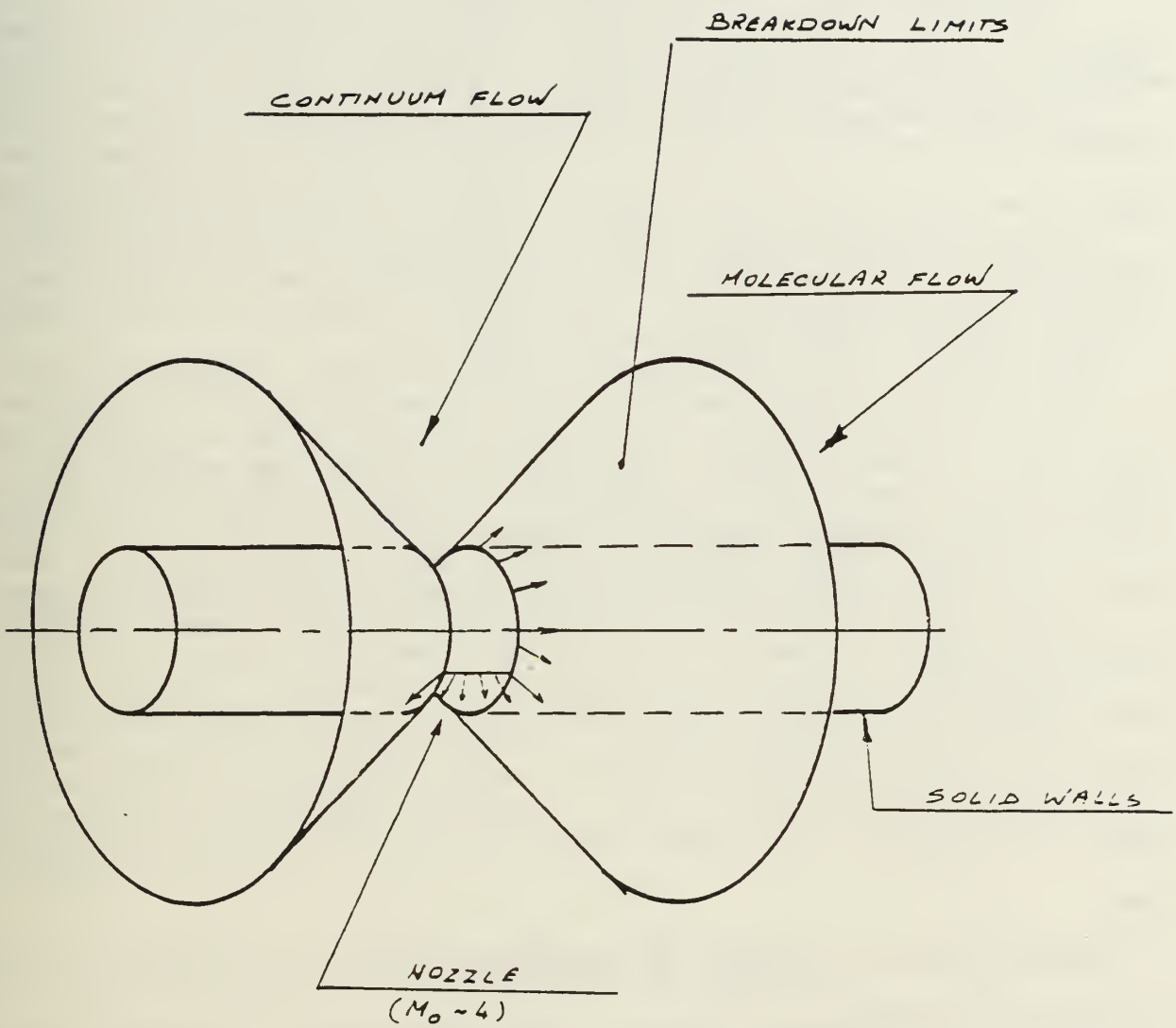


Figure 12. Regions in a ring jet.

predict how far the simulated results will be from the exact solutions. These comparisons have to be made after getting final results of this simulation.

1. The Direct Simulation Monte Carlo Method

The direct simulation Monte Carlo Method is a technique for a computer modeling of a real gas by some thousands of simulated molecules. The velocity components and the coordinates of the simulated molecules are stored in the computer and are modified with time as a result of collisions and boundary interactions. A detailed description of some problems and their solutions by means of direct simulation is given in [4].

To follow the molecular motion it is necessary to divide the simulated domain into a network of cells. The size of a cell must be such that the change in flow properties across each cell is small. The time is advanced in discrete steps DTM, such that DTM is small compared with the mean collision time per molecule. If there is a flow going through the domain, DTM should be small compared with the mean time required for the mean flow to cross the cells.* Both cell size ((DR),(DDALFA) - radial size and angular size as they appear in the program) and DTM may vary in the simulation with position and time.

Applications such as free jet expansion in which large gradients of flow properties are expected, may require a very large number of cells for the simulation. In these cases the computer memory requirements to store cells' data and molecules' data may exceed the available computer storage. A

*If DTM is chosen to be very small compared with the mean time between collisions then the simulation will require a very large number of runs such that the number of collisions will be sufficient. If DTM is large the molecules are washed out by the mean flux and there is no time for the collisions to influence the flow.

solution for this problem is to divide the simulation space into smaller regions and to run the simulation for each region separately. If there is an interaction between different regions, which apriori is undefined, the solution should be found iteratively. (That means that each run will provide data for consecutive runs and the procedure should be repeated until the results converge to a steady solution.

The computation of a representative set of collisions based on mean collision time per molecule is invalid for a computerized simulation because of the large computer time and computer memory requirements. Instead, the method proposed by Derzko which is described in details by Bird [4] may be employed. Following this method, an averaged mean time between collisions of species L with species M for a cell is calculated. The number of collisions of each type (L.M species) is such that the collision time counters are kept concurrent with the overall time parameter. The L.M collision time for a cell containing N_L and N_M molecules with collision cross section σ_{LM}, number densities n_L and n_M and relative velocity C_r, is given by

$$\Delta t_c = \frac{LP}{N_L} \frac{1}{\sigma_{LM} n_M C_r} + \frac{MP}{N_M} \frac{1}{\sigma_{LM} n_L C_r} \qquad (12)$$

where LP and MP are the probabilities that the collision will be effective for the L and M molecules respectively.

B. THE GEOMETRY OF THE SIMULATED DOMAIN, SECTORS, REGIONS AND CELLS

Figure (13) shows a cross section of the simulated domain for the axisymmetric (ring) flow. Points A and A' are the nozzle lips. Starting at "A" and assuming the "breakdown" boundary to be a straight line, we obtain the cross section of the molecular domain as a sector defined by LAM. The solid wall is defined by AL. The arc LM may be assumed to be far enough so that the pressure along it may be assumed to equal the ambient pressure. Molecules originated in the jet cross the breakdown boundary with a velocity, direction, temperature (and other thermodynamic properties) as found from the continuum solution.

The molecular domain LAM is divided into secondary sectors, and each of these are divided into several radial regions making the "simulation regions".

Because we have no apriori information on how the expansion occurs, the angle of each sector (which mainly is in the direction of the expansion gradients) is left to be a result of the internal calculation.

Each region is divided into NRD radial divisions and NAD angular divisions making a network of NAD*NRD simulation cells. The angle DALFA of all regions in a sector is constant. Taking NAD constant for all regions in a sector, we get the angle of a cell DDALFA constant. Defining the radial size of a cell DR as constant we get a cell cross section area proportional to the radius R measured from the nozzle lip (point A).

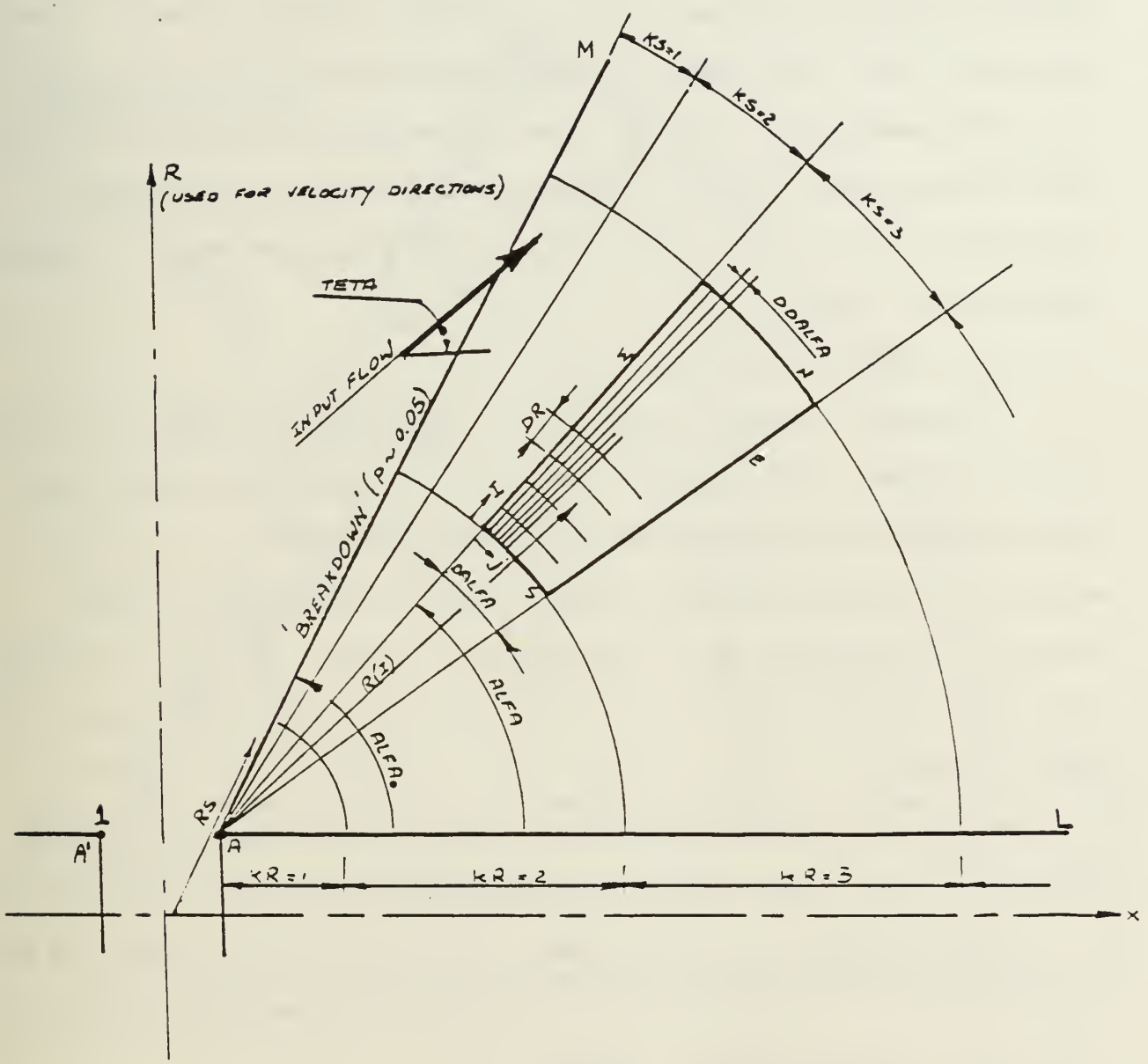


Figure 13. Cross section of the simulation domain, definition of sectors, regions, cells and coordinates.

The size of a cell: In order to get accurate simulated results it is recommended to define the size of a cell (DR and R*DDALFA) small compared with the mean free path of the molecules λ (typical DR=λ/3). However, as we do not expect to get large changes in flow parameters along the radius we may allow DR be much larger than $\lambda/3$. The angular size of the largest cell in a sector should comply with this requirement, but because of the computer limitation it is set to be equal to $5*\lambda$. This will be the basis for defining DALFA for each sector.

C. INITIAL NUMBER OF MOLECULES IN CELLS

A "reasonable" number of molecules in a simulation is several thousands (a larger number, which is better, may be used for simple problems or when using a single user computer with large user memory space). The initial setting of molecules in cells is usually based on a guess of the number density in the specific cell. (The number of molecules in cells will change during the simulation according to the input/output calculated fluxes to the specific region).

The number density and the size of a cell are specified only in three dimensional flows. When applied to a two dimensional flow the simulation may be regarded as applying to an arbitrary thin slice of the real flow. In the axisymmetric flow we define the width of a cell by the angle DFI as shown in Figure (14), constant within a region.

The initial number density in cells of a given region is set constant. Defining the total number of simulated molecules in the region the number of molecules in each specific cell becomes a function of DFI. For example, assume that we limit the number of molecules in the smallest cell in the region to 15 then:

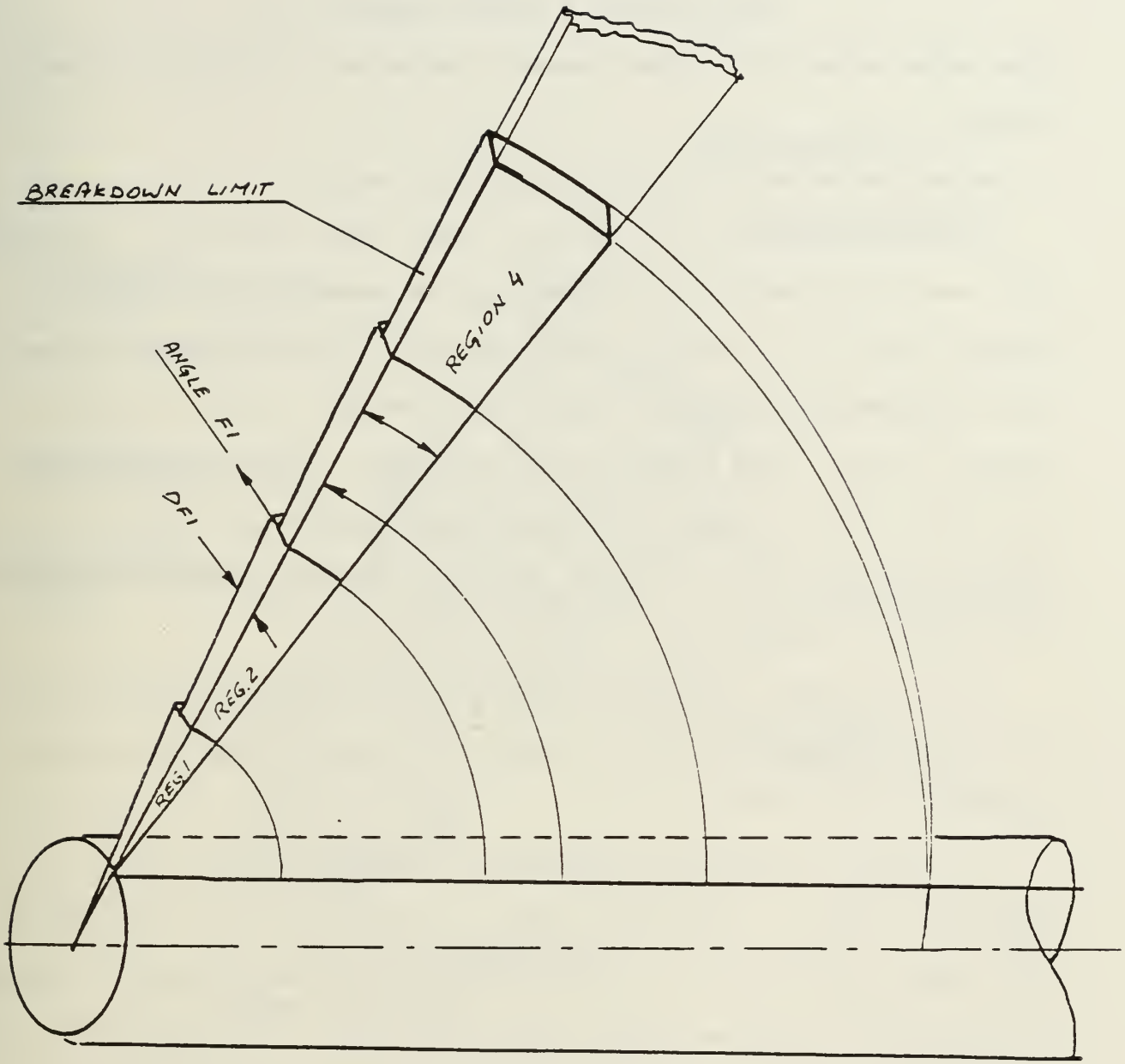


Figure 14. Variation of the angle DFI.

To maintain the number of simulated molecules within computational limits, the 'width' of each region defined by DFI is such that:

MIN = number of molecules in smallest cell in a region
MIN = VOLUME (smallest cell) * number density
= f(R, ALFA, DALFA) * DFI * number density for flux calculations

DFI is a weighting factor.

DFI*(contant) * (number density) = 15

Other cells contain the initial number of molecules proportional to their volumes.

D. DEFINITION OF INPUT AND OUTPUT FLOWS FOR A REGION

The cross sections of all regions (except those regions near the nozzle lips) are quadrilateral. Through the sides of the region molecules are allowed to enter or to leave according with the boundary conditions or as a result of molecular velocity. For the first sector, near the breakdown boundary the input flow (FWP1 and FWP2 see Figure (15)) is defined by the results from the continuum flow. FEN1, FNN1, FSN1, etc. are results of counting and averaging the outgoing molecules (the different vector names will be explained in Appendix B).

For the neighbor regions these output fluxes become inputs and have to be adjusted according to the differences in the angle DF1 of the different regions.

The simulation starts with regions in the sector near the breakdown boundary. At this time there is no data for input flows through faces E and N of the cell. An additional run of the whole program is required in order to take these calculated flows into account. If the accuracy of the results is important we may run this type of iteration several times until the results become stable. (Only after running the program for the whole domain once we shall be able to evaluate the importance of these iterations.)

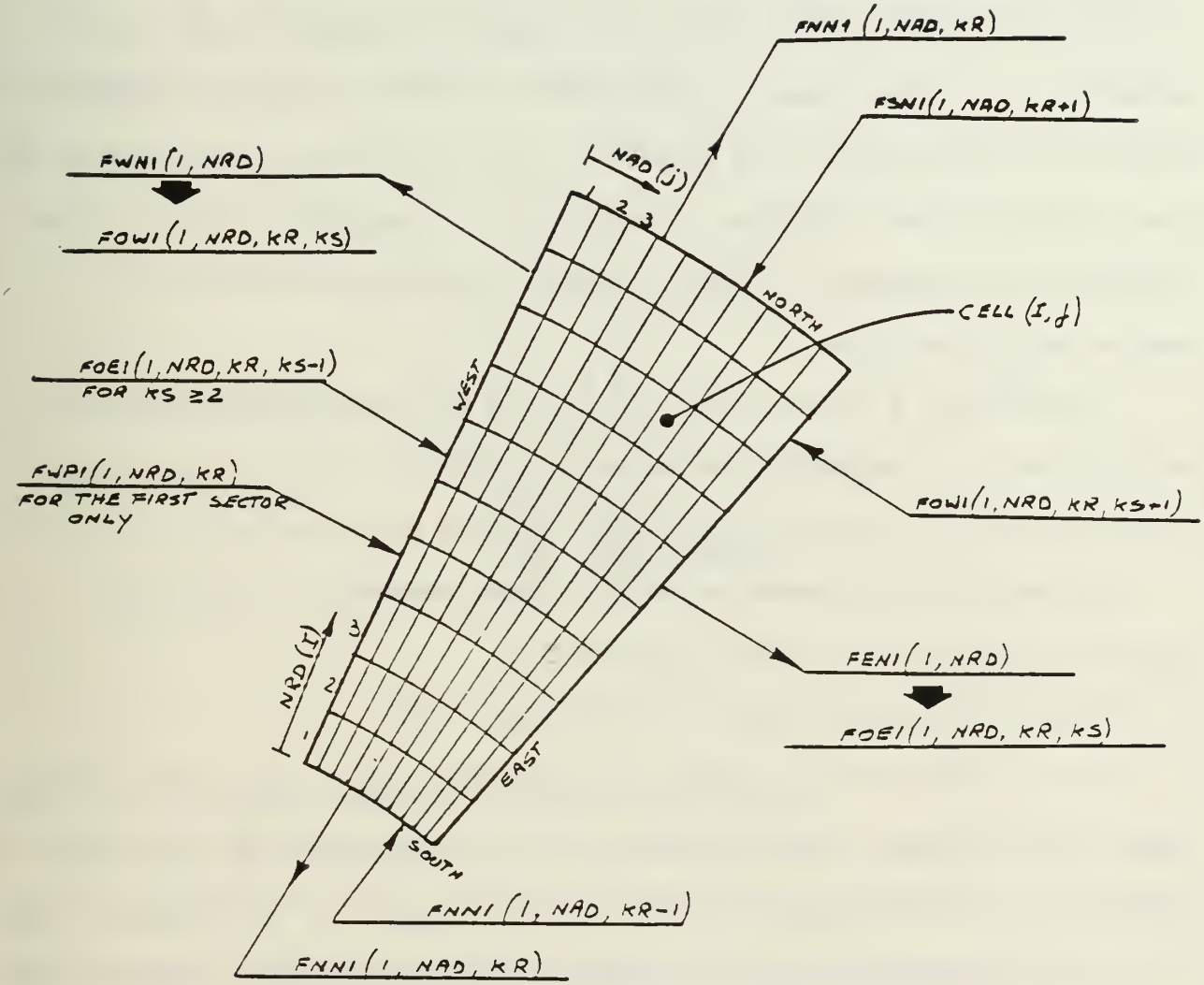


Figure 15. Definition of input and output flows of species 1 to a region (KR) in a sector (KS).

(For species 2 the flux names will change as follows:
instead FWN1( ) → FWN2( )
instead FOW1( ) → FOW2( )
etc.

E. COLLISIONLESS FLOW

In several sectors near the breakdown boundary we may find a high number density and the mean free path small compared with the size of a cell. There the calculated collisions are expected to have an influence on the flow parameters. For wider expansion angles the collisions become rare mainly because of the decrease in the density. In the ambient gas the mean free path (for 200 km altitude) is 240 m. Comparing this number with the size of the simulated domain may lead to the conclusion that there the flow may be regarded as collisionless.

We may define a limiting line in the flow where the collisions become insignificant. Consequently, molecules crossing this limit will in fact continue moving in straight lines; a part of them reach the solid wall.

Introducing this idea of the collisionless flow we may reduce the computation time and the memory requirements.

F. TWO DIMENSIONAL PLANAR FLOW VS. AXISYMMETRIC FLOW

The cell dimensions are completely specified only in three dimensional flow. When applied to two dimensional flow, the simulation may be regarded as applying to an arbitrarily thin slice of the real flow. The thickness of the slice may be chosen such that the number of simulated molecules complies with the cell volume and the physical number density. For the axisymmetric flow we have defined the angle DFI as the third coordinate so that the volume of the cell is completely specified.

Once the geometry is defined, the simulation may be accomplished and there is no difference if doing it for two dimensional or for axisymmetric flows.

APPENDIX A - THE AXSYM PROGRAM

A.1 DIFFERENT REGIONS IN THE JET

For the two dimensional jet with initial Mach number greater than unity the different regions are shown in Figure (16).

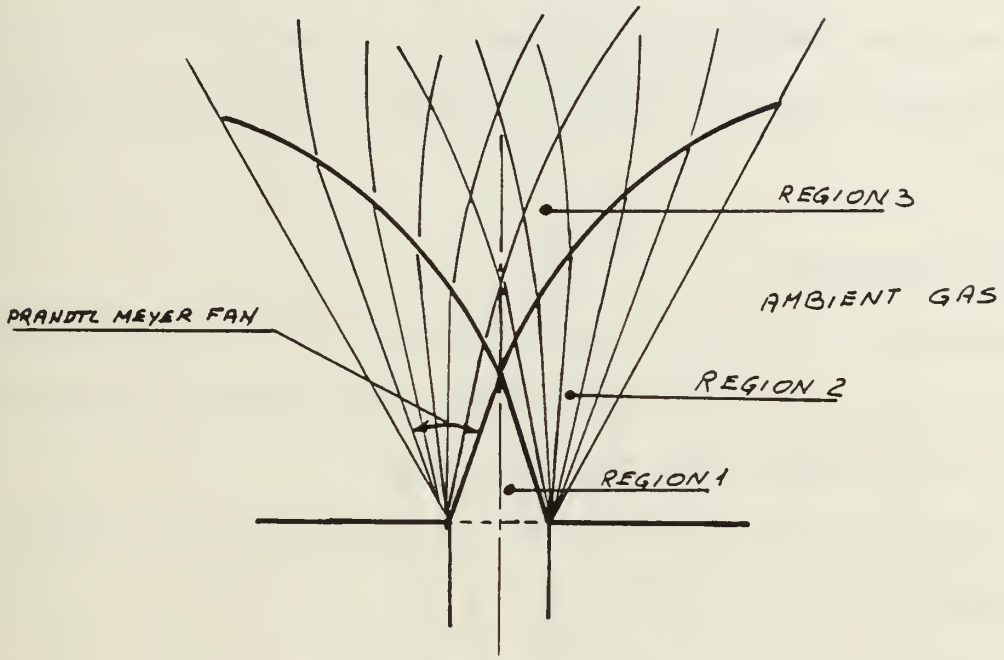


Figure 16. The three regions in an underexpanded jet.

For planar 2-D flow region 1 is a uniform flow core, region 2 is a simple region in which only one family of characteristics define the flow, and region 3 which contains the intersection of the two families of characteristics. Because our intention is to find solutions for highly underexpanded jets with very low ambient pressure, the calculation of further downstream flow is not necessary.

For the axisymmetric ring jet, we use the same definition for the different regions however, in this case none of the three regions has uniform flow and is not a simple region.

As shown in Equations (9,10) the PM function (ν) and the flow direction (θ) of a point at location I,j may be calculated from the ν and θ of two upstream points (I-1,j) and (I,j-1). Later, from the PM function at the new point we may derive the local Mach number, the local pressure, temperature, velocity and other thermodynamic parameters as required.

Definition of the mesh of points for the different regions is shown in Figure (17).

A.2 PROGRAM FLOWCHART

A simplified flowchart for the MOC program is shown in Figure (18). The program is designed to solve both axisymmetric as well as two dimensional flow

for kD = 2 it solves two dimensional flow

for kD = 3 it solves axisymmetric flow (This is also the default condition)

Initial data such as Mach number and pressure at the exit surface, ambient pressure and jet gas parameters are input data.

Output data contains the following for each mesh point:

Mach number, coordinates of mesh point (R,X), flow direction (TETA), pressure, temperature, local velocity, Knudsen number based on the distance between two points along a streamline, mean free path and breakdown parameter as defined by Bird.*

For each of the three regions, we start with precalculated boundary conditions enabling the calculation of the Mach angles, coordinates of mesh points and distances $d\xi$ and $d\eta$ as described in [2].

*For the exit plane instead the Bird's breakdown parameter, we calculate the ratio between time per three collisions and time of motion. Sometimes this ratio may be regarded as a measure of the breakdown of the continuum theory.

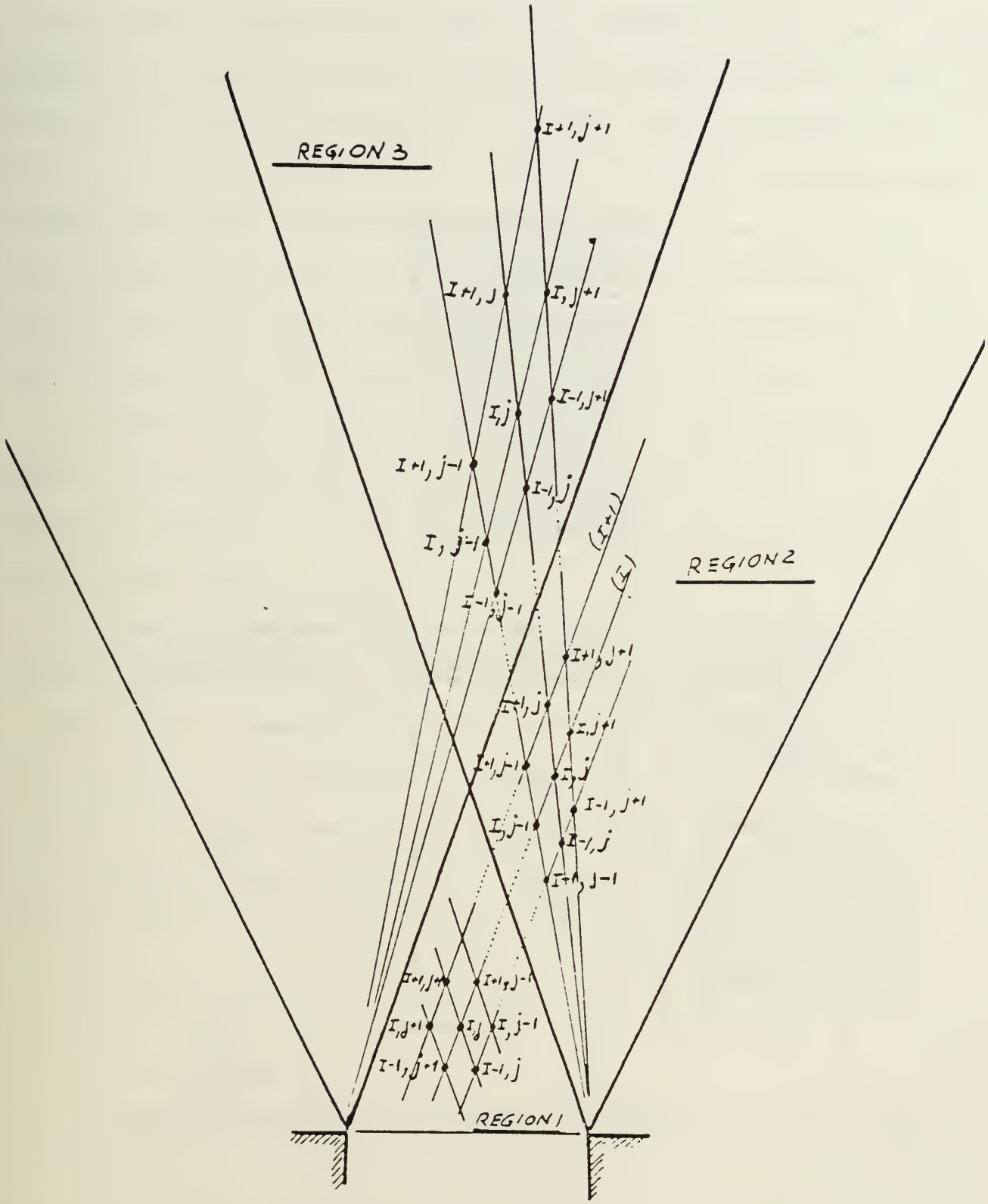


Figure 17. Indexing of mesh points for the different regions in the 'AXSYM' program.

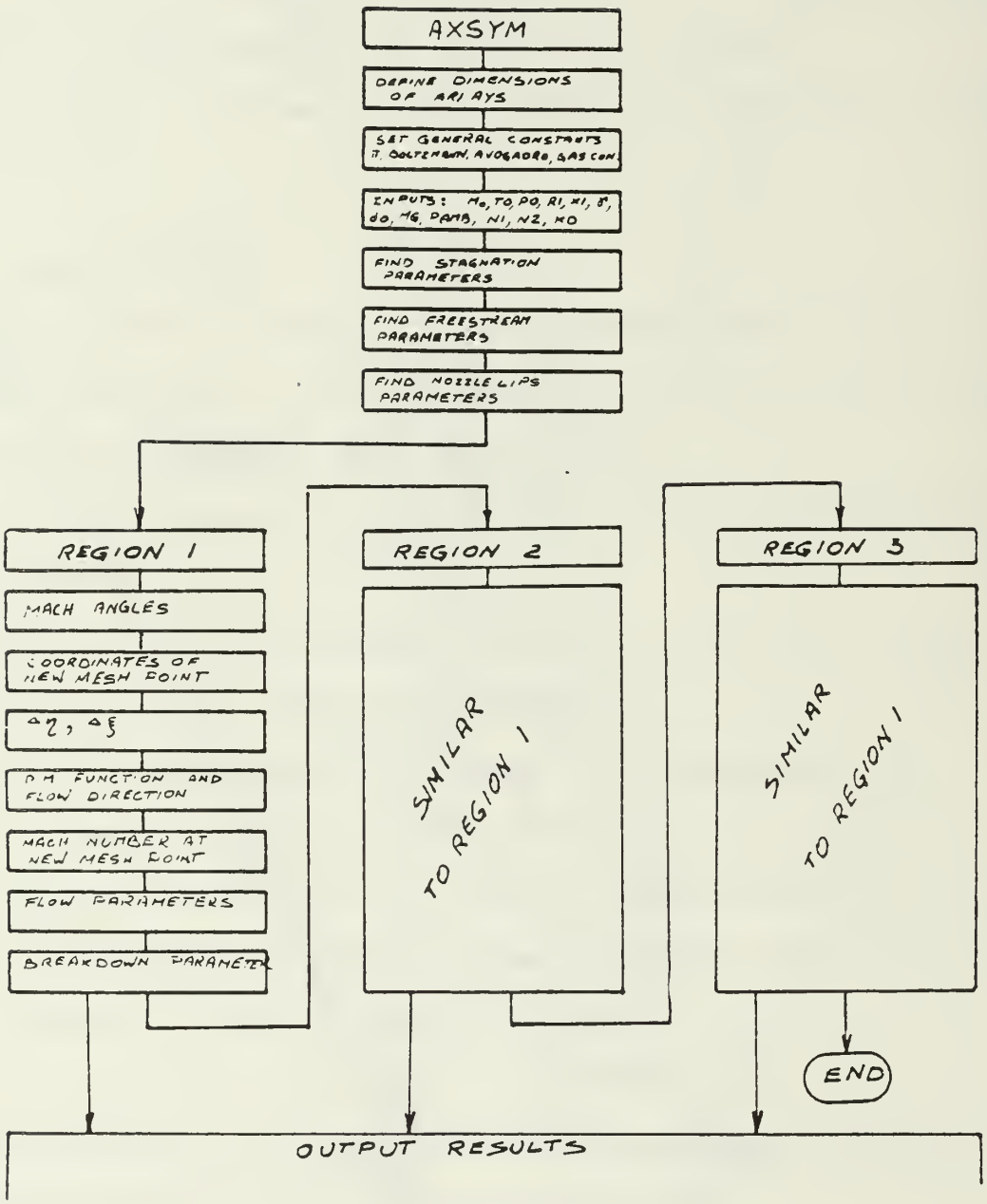


Figure 18. AXSYM Program Flowchart

The number of characteristics used in the program is arbitrary and depends on the required resolution (it may affect also the accuracy of the results and the amount of computation). We start with 20 characteristics along the exit cross section and with 50 characteristics in the Prandtl-Meyer fan thus a total of 70 characteristics of each family are calculated. In region 1 there are 20 left running and 20 right running characteristics. In region 2 there are 20 right running and 50 left running characteristics. In region 3 there are 50 left running and 50 right running characteristics.

In region 3 we limit the calculation where the two characteristics defining a new mesh point intersect at an angle smaller than the computational accuracy. In fact this occurs far downstream where continuum theory becomes invalid.

After defining the mesh geometry (successively) we calculate the Prandtl-Meyer function and flow direction, using equations (9,10).

The local Mach number is an implicit function of the Pradtl-Meyer angle. It is calculated by iterations with an initial guess of local Mach number set equal to a precalculated Mach number at an adjacent point, and the slope of the function as given by Equation (5). Figure (19) shows the iterative procedure for evaluating the Mach number at each mesh point.

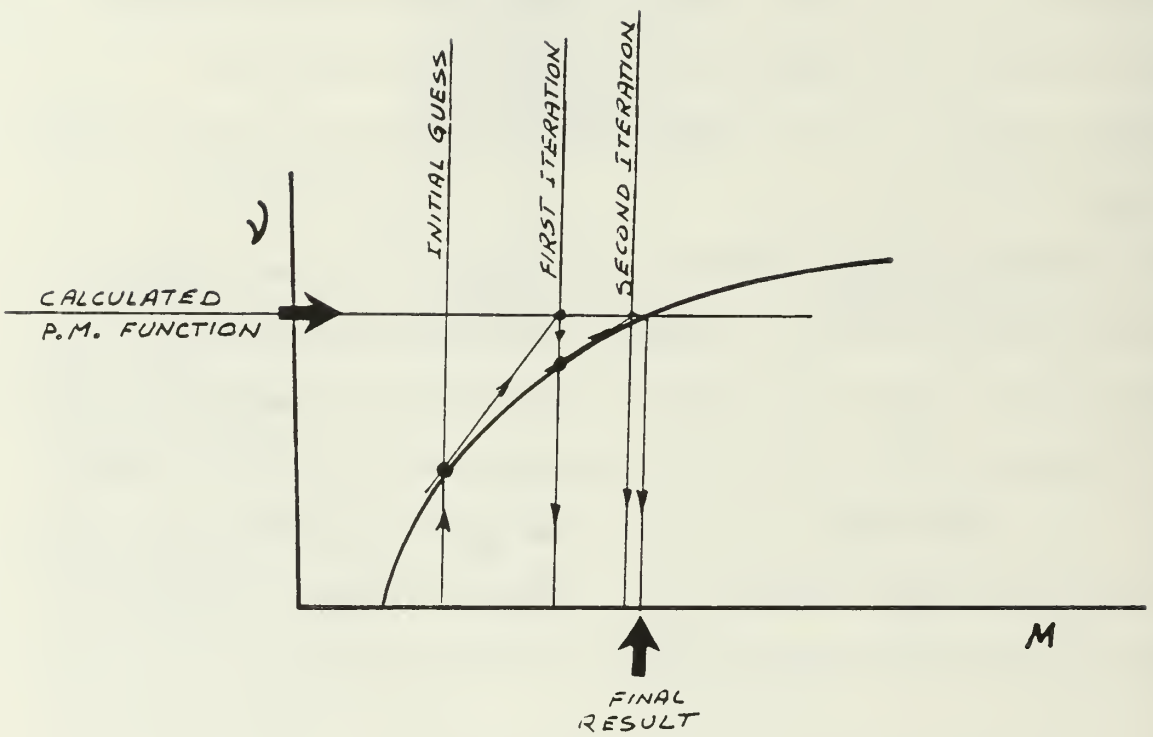


Figure 19. Iterative procedure for Mach number calculation.

Once the local Mach number has been found all other flow parameters may be defined using the Equation (1,2,3).

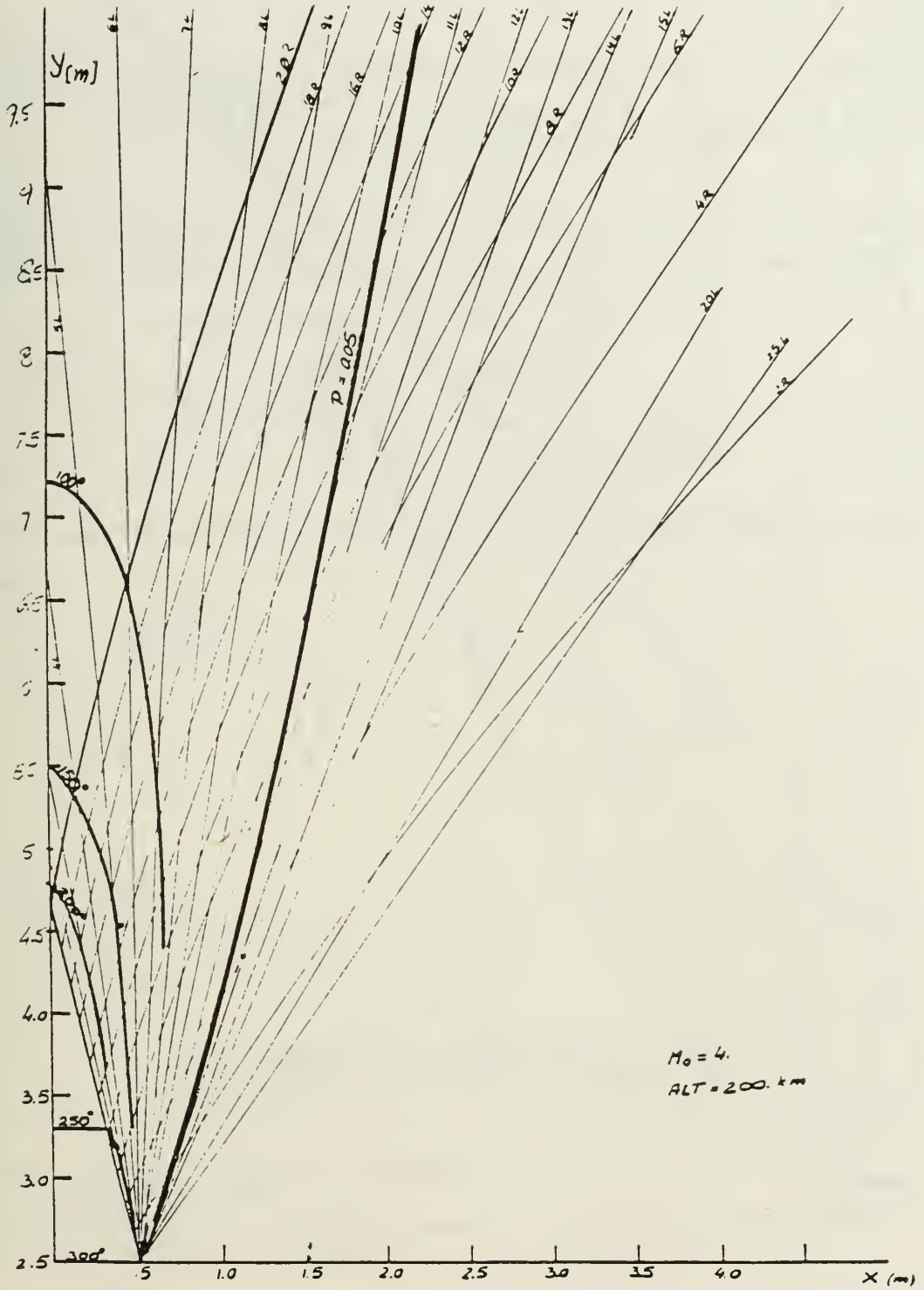


Figure 20. The mesh of characteristics in Region 2 and Region 3

Axisymmetric ring jet. M_0 = 4. Altitude=200km.

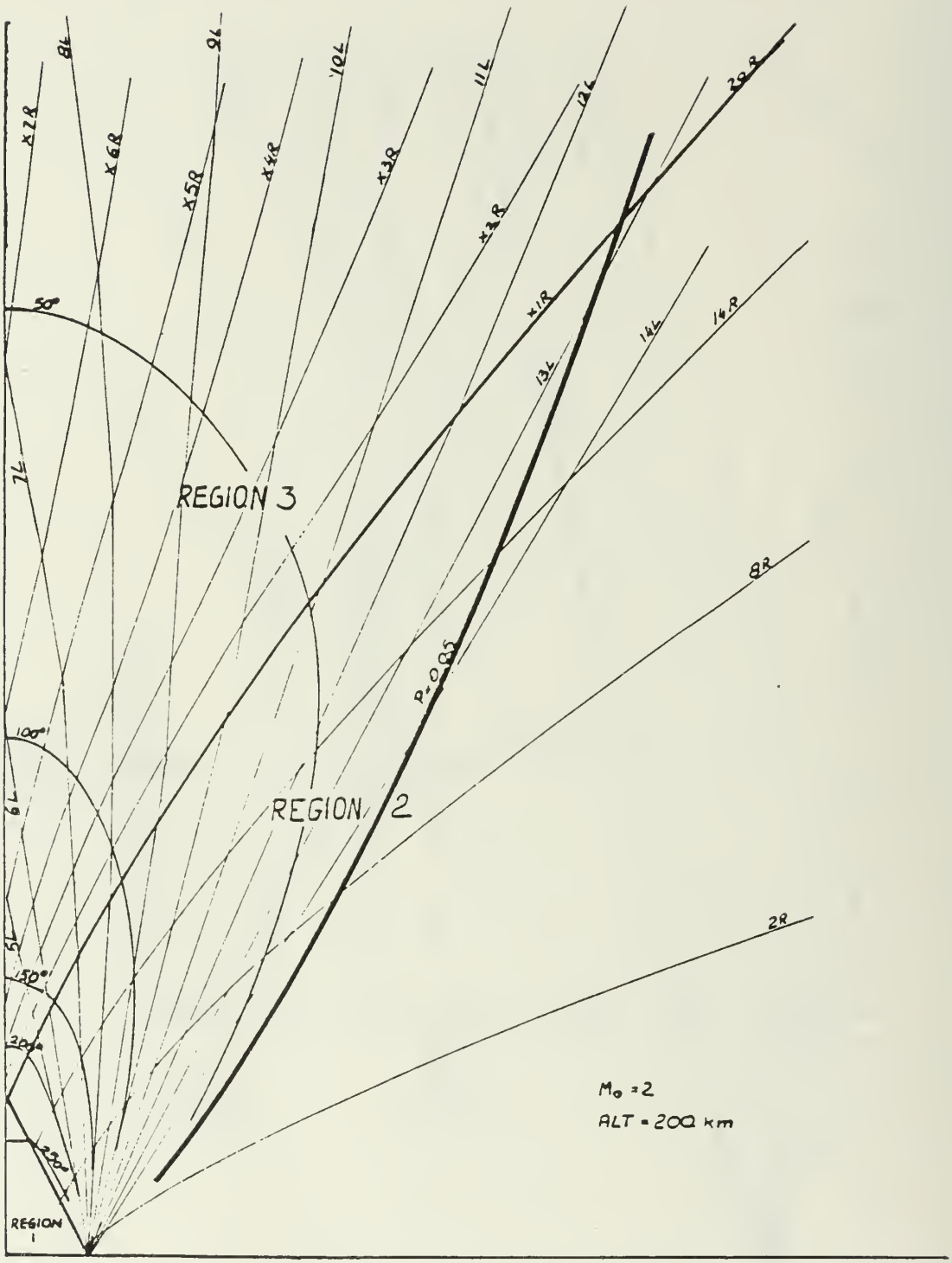


Figure 21. The mesh characteristics in Region 2 and Region 3

Axisymmetric ring jet. M_o = 2. Altitude = 200km.

A.3 PROGRAM 'AXSYM' LISTING

```
$JOB                                                                    AXS00010
C  PROGRAM AXSYM                                                       AXS00020
C                                                                       AXS00030
C  THIS PROGRAM CALCULATES THE ISENTROPIC EXPANSION OF A JET BY MEANS OFAXS00040
C  THE METHOD OF CHARACTERISTICS.                                       AXS00050
C        FOR A TWO DIMENSIONAL    JET 'KD' SHOULD BE SET EQUAL TO 2     AXS00060
C        FOR AN AXISYMMETRIC RING JET 'KD' SHOULD BE SET EQUAL TO 3     AXS00070
C                                                                       AXS00080
      IMPLICIT REAL*8(A-H,O-Z,$)                                        AXS00090
      DIMENSION TETA(20,50),AM(20,50),R(20,50),X(20,50),PM(20,50)       AXS00100
      DIMENSION AMCOR(20,20),TETAC(20,20),XC(20,20),RC(20,20),PMC(20,20)AXS00110
      DIMENSION DENSF(20,50)                                            AXS00120
      DIMENSION AMX(50,50),TETAX(50,50),XX(50,50),RX(50,50),PMX(50,50)  AXS00130
C                                                                       AXS00140
C TETA IS THE FLOW ANGLE (RADIANS) MEASURED FROM X AXIS.                AXS00150
C AM IS THE MACH NUMBER                                                 AXS00160
C R IS THE RADIUS           (NORMAL TO THE WALL)                        AXS00170
C X IS THE AXIAL LOCATION   (PARALLEL TO THE WALL)                       AXS00180
C PM IS THE PRANDTL MEYER FUNCTION                                      AXS00190
C***********************************************************************AXS00200
C THE FOLLOWING IS DATA FOR THE SPECIFIC PROBLEM                        AXS00210
      PAMB = 8.4736E-5                                                  AXS00220
      KD = 3                                                            AXS00230
C FOR TWO DIMENSIONAL FLOW KD=2 ,FOR AXISYMMETRICAL FLOW KD=3           AXS00240
C***********************************************************************AXS00250
C                                                                       AXS00260
C CONSTANTS                                                             AXS00270
      PI    = 3.141593                                                  AXS00280
      BOLTZ = 1.38032E-23                                               AXS00290
      AVOG  = 6.0225E+26                                                AXS00300
      RG    = 8314.3                                                    AXS00310
C EXIT SURFACE                                                          AXS00320
      AM0 = 4.00                                                        AXS00330
      T0  = 300.0                                                       AXS00340
      P0  = 136.0                                                       AXS00350
C                                                                       AXS00360
      R1  = 2.5                                                         AXS00370
      X1  = 0.5                                                         AXS00380
C                                                                       AXS00390
C GAS DATA                                                              AXS00400
      GAMA = 1.535                                                      AXS00410
      DIAM = 2.95E-10                                                   AXS00420
      GM   = 17.0                                                       AXS00430
      RJ = RG/GM                                                        AXS00440
      CXS = PI*DIAM*DIAM                                                AXS00450
      GMM = GM/AVOG                                                     AXS00460
C                                                                       AXS00470
C MESH DEFINITION                                                       AXS00480
C                 N1=CHARACTERISTICS FROM THE EXIT PLANE                AXS00490
C                 N2=CHARACTERISTICS FROM THE CORNERS                   AXS00500
      N1 = 20                                                           AXS00510
      N2 = 50                                                           AXS00520
C                                                                       AXS00530
C CONSTANTS FOR THE ISENTROPIC EXPANSION                                AXS00540
      A1 = (GAMA-1.0)/GAMA                                              AXS00550
      B1 = 1.0/A1                                                       AXS00560
C                                                                       AXS00570
      A2 =DSQRT((GAMA+1.)/(GAMA-1.))                                    AXS00580
      B2 = 1.0/A2                                                       AXS00590
C                                                                       AXS00600
      A3 = (GAMA-1.)/2.                                                 AXS00610
C                                                                       AXS00620
C     C = MACH*MACH*A3 + 1.                                             AXS00630
C     D = MACH*MACH -1.                                                 AXS00640
C***********************************************************************AXS00650
C***********************************************************************AXS00660
C                                                                       AXS00670
C DEFINE STAGNATION PARAMETERS                                          AXS00680
C                                                                       AXS00690
C***********************************************************************AXS00700
      C = (1.0+A3*AM0*AM0)                                              AXS00710
C PRESSURE                                                              AXS00720
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```
      PN = C**B1                                                        AXS00730
      PSTG = P0*PN                                                      AXS00740
C TEMPERATURE                                                           AXS00750
      TSTG = T0*C                                                       AXS00760
C DENSITY                                                               AXS00770
      D0 = P0/(RJ*T0)                                                   AXS00780
      DSTG = PSTG/(RJ*TSTG)                                             AXS00790
C                                                                       AXS00800
C**************                                                        AXS00810
      WRITE(6,1)PSTG,TSTG,DSTG,DIAM,GM                                  AXS00820
    1 FORMAT('0','STAGNATION   PRESSURE=',E12.5,'   TEMPERATURE=',F10.5,AXS00830
     1'   DENSITY=',E12.5,'   MOL.DIAM=',E12.5,'   MOL.MASS=',F10.5)    AXS00840
      WRITE (6,2)P0,T0,D0,AM0                                           AXS00850
    2 FORMAT('0','EXIT PLANE   PRESSURE=',E12.5,'   TEMPERATURE=',F10.5,AXS00860
     1'   DENSITY=',E12.5,'   MACH=',F10.5)                             AXS00870
C*****************************************************************************AXS00880
C*****************************************************************************AXS00890
C                                                                       AXS00900
C DEFINE FREE STREAM PARAMETERS AT THE RIGHT CORNER                     AXS00910
C                                                                       AXS00920
C*****************************************************************************AXS00930
C MACH NUMBER                                                           AXS00940
      FSM = DSQRT(((PSTG/PAMB)**A1-1.)/A3)                              AXS00950
C TEMPERATURE                                                           AXS00960
      FST = TSTG/(1.+A3*FSM*FSM)                                        AXS00970
C DENSITY                                                               AXS00980
      FSD = PAMB/(RJ*FST)                                               AXS00990
C MACH ANGLES FOR HEAD AND TAIL OF FAN                                  AXS01000
      AMIT =DARSIN(1./AM0)                                              AXS01010
      AMIH =DARSIN(1./FSM)                                              AXS01020
C PRANDTL MEYER FUNCTION FOR HEAD AND TAIL OF FAN                       AXS01030
      D1 =DSQRT(AM0*AM0-1.)                                             AXS01040
      D2 =DSQRT(FSM*FSM-1.)                                             AXS01050
      PMH = A2*DATAN(B2*D2)-DATAN(D2)                                   AXS01060
      PMT = A2*DATAN(B2*D1)-DATAN(D1)                                   AXS01070
C EXTERNAL TURNING ANGLE (FREE STREAM ANGLE)=EXTA                       AXS01080
      EXTA = PMH - PMT                                                  AXS01090
C PRANDTL MEYER FAN ANGLE PMFA                                          AXS01100
      PMFA = EXTA - AMIH + AMIT                                         AXS01110
C                                                                       AXS01120
C**************                                                        AXS01130
C     WRITE(6,3)PAMB,FST,FSD,FSM                                        AXS01140
C   3 FORMAT('0','FREE STREAM  PRESSURE=',E12.5,'   TEMPERATURE=',F10.5,AXS01150
C    1'   DENSITY=',E12.5,'   MACH=',F10.5///)                          AXS01160
C*****************************************************************************AXS01170
C*****************************************************************************AXS01180
C                                                                       AXS01190
C DEFINE THE MESH OF CHARACTERISTICS-AND FLOW PARAMETERS                AXS01200
C                                                                       AXS01210
C*****************************************************************************AXS01220
C THE CORNER POINT - LEFT RUNNING CHAR.                                 AXS01230
C PMFA IS DEVIDED INTO N2 (=50) NONEQUAL DIVISIONS                      AXS01240
C                                                                       AXS01250
      RAT = (FSM/AM0-1)/0.02                                            AXS01260
      RAT2 = FLOAT(N2-1)                                                AXS01270
      E1 = DLOG(RAT)/DLOG(RAT2)                                         AXS01280
C                                                                       AXS01290
      WRITE(6,4)                                                        AXS01300
    4 FORMAT('1','PRANDTL MEYER FAN          LINE          MACH         AXS01310
     1      P.M. ANGLE        TETA'/)                                   AXS01320
      DO 20 N=2,N2                                                      AXS01330
      EN2 = FLOAT(N-2)                                                  AXS01340
      EN1 = FLOAT(N-1)                                                  AXS01350
      AMB = AM0*(1.+.02*(EN2)**E1)                                      AXS01360
      AMF = AM0*(1.+.02*(EN1)**E1)                                      AXS01370
      DELM = AMF-AMB                                                    AXS01380
      AM(1,N) = AMF                                                     AXS01390
      D1 =DSQRT(AM(1,N)*AM(1,N)-1.)                                     AXS01400
      PM(1,N) = A2*DATAN(B2*D1)-DATAN(D1)                               AXS01410
      AMI =DARSIN(1./AM(1,N))                                           AXS01420
      TETA(1,N) = PI/2.-(PM(1,N)-PMT)                                   AXS01430
C TETA IS THE FLOW ANGLE ON THE CHARACTERISTICS AT THE CORNER           AXS01440
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      R(1,N) = R1                                                       AXS01450
      X(1,N) = X1                                                       AXS01460
      ALFAL = TETA(1,N)+AMI                                             AXS01470
C ALFAL IS THE ANGLE OF THE LEFT RUNNING CHARACTERISTICS                AXS01480
C                                                                       AXS01490
C PRESSURE, TEMPERATURE AND DENSITY VARIATION AT THE CORNER             AXS01500
      C = AM(1,N)*AM(1,N)*A3+1.                                         AXS01510
      PRES = PSTG/(C**B1)                                               AXS01520
      TEMP = TSTG/C                                                     AXS01530
      DENSF(1,N) = PRES/(RJ*TEMP)                                       AXS01540
C                                                                       AXS01550
C********                                                               AXS01560
      WRITE (6,5) N,AM(1,N),PM(1,N),TETA(1,N)                           AXS01570
    5 FORMAT(' ','                              ',1I5,3E20.5)           AXS01580
C********                                                               AXS01590
   20 CONTINUE                                                          AXS01600
C                                                                       AXS01610
C***********************************************************************AXS01620
C                                                                       AXS01630
C***********************************************************************AXS01640
      WRITE(6,10)                                                       AXS01650
   10 FORMAT('0','   I   J      MACH        R          X       TETA     AXS01660
     1TEMP      PRESS    VELOCITY      KNUDSEN     MFP        ND        AXS01670
     1   P')                                                            AXS01680
C                                                                       AXS01690
C                                                                       AXS01700
C***********************************************************************AXS01710
C***********************************************************************AXS01720
C                                                                       AXS01730
C DEFINE THE PARAMETERS AT THE EXIT SURFACE (PLANE)                     AXS01740
C                                                                       AXS01750
C***********************************************************************AXS01760
      DO 25 J = 1,N1                                                    AXS01770
      AMCOR(1,J) = AM0                                                  AXS01780
      D = DSQRT(AM0*AM0-1.)                                             AXS01790
      PMC(1,J) = A2*DATAN(B2*D)-DATAN(D)                                AXS01800
   25 TETAC(1,J) = PI/2.                                                AXS01810
C                                                                       AXS01820
C THE EXIT PLANE IS DIVIDED INTO (N1-1) DIVISIONS (N1 POINTS)           AXS01830
      DO 30 J=1,20                                                      AXS01840
      SOUND = DSQRT(GAMA*RJ*T0)                                         AXS01850
      VEL0 = AMCOR(1,J)*SOUND                                           AXS01860
      DN0 = P0/(BOLTZ*T0)                                               AXS01870
      FP0 = .707/(DN0*CXS)                                              AXS01880
      DX = X1*2./FLOAT(N1)                                              AXS01890
      AKN0 = FP0/DX                                                     AXS01900
C                                                                       AXS01910
      XC(1,J) = X1*(1.-FLOAT(J-1)/FLOAT(N1-1)*2.)                       AXS01920
      CENTR = DABS(XC(1,J))                                             AXS01930
      IF(CENTR.LT.0.001) XC(1,J) = 0.                                   AXS01940
      RC(1,J) = R1                                                      AXS01950
C                                                                       AXS01960
C.........................                                              AXS01970
C     KZ=1*******************                                          AXS01980
      IF (J.GT.1) GO TO 29                                              AXS01990
C AT THE EXIT PLANE THE BREAKDOWN PARAMETER IS EVALUATED BY MEANS OF    AXS02000
C THE RATIO OF THE COLLISION TIME AND THE FLOW TIME. LENGTH SCALE IS    AXS02010
C THE MESH DIMENSION.                                                   AXS02020
      SCALE = DX*DTAN(DARSIN(1./AM0))/2.                                AXS02030
      TIME1 = SCALE/VEL0                                                AXS02040
      TIME2 = 3./(4.*CXS*DN0*DSQRT(BOLTZ*T0/(PI*GMM)))                  AXS02050
      P =TIME2/TIME1                                                    AXS02060
      DENSF(1,1) = D0                                                   AXS02070
   29 CONTINUE                                                          AXS02080
C                                                                       AXS02090
      WRITE(6,11)1,J,AMCOR(1,J),R1,XC(1,J),TETAC(1,J),T0,P0,VEL0,AKN0,FPAXS02100
     10,DN0,P                                                           AXS02110
   11 FORMAT(' ',2I4,5F10.3,3E12.3,F9.4,2E12.3)                         AXS02120
   30 CONTINUE                                                          AXS02130
C                                                                       AXS02140
C***********************************************************************AXS02150
C***********************************************************************AXS02160
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C                                                                       AXS0217
C CALCULATE THE FLOW PARAMETERS IN THE CORE BOUNDED BY THE TWO MACH     AXS0218
C WAVES STARTING AT THE NOZZLE LIPS (CORNER POINTS)                     AXS0219
C AT THE EXIT THE FLOW IS ASSUMED TO BE UNIFORM                         AXS0220
C                                                                       AXS0221
C***********************************************************************AXS0222
      WRITE (6,198)                                                     AXS0223
  198 FORMAT('1','   CORE    '/)                                        AXS0224
      APM=0.                                                            AXS0225
      BPM=0.                                                            AXS0226
      CPM=0.                                                            AXS0227
C                                                                       AXS0228
      DO 199 I = 2,N1                                                   AXS0229
      WRITE (6,10)                                                      AXS0230
      DO 199 J = 1,N1                                                   AXS0231
      IF ((I+J-1).GT.N1) GO TO 199                                      AXS0232
      AMIL = DARSIN(1./AMCOR(I-1,J))                                    AXS0233
      ALFAL = PI-(TETAC(I-1,J)+AMIL)                                    AXS0234
C                                                                       AXS0235
      AMIR = DARSIN(1./AMCOR(I-1,J+1))                                  AXS0236
      ALFAR = TETAC(I-1,J+1)-AMIR                                       AXS0237
C                                                                       AXS0238
      XC(I,J) = (RC(I-1,J)-RC(I-1,J+1)+XC(I-1,J)*DTAN(ALFAL)+XC(I-1,J+1)AXS0239
     1*DTAN(ALFAR))/(DTAN(ALFAL)+DTAN(ALFAR))                           AXS0240
      CENTR = DABS(XC(I,J))                                             AXS0241
      IF (CENTR.LT.0.001) XC(I,J) = 0.                                  AXS0242
      RC(I,J) = RC(I-1,J+1)+(XC(I,J)-XC(I-1,J+1))*DTAN(ALFAR)           AXS0243
C                                                                       AXS0244
      DKSI = DSQRT((XC(I,J)-XC(I-1,J+1))**2+(RC(I,J)-RC(I-1,J+1))**2)   AXS0245
      DETA = DSQRT((XC(I,J)-XC(I-1,J))**2+(RC(I,J)-RC(I-1,J))**2)       AXS0246
C                                                                       AXS0247
C                                                                       AXS0248
C CALCULATE NOW THE PRANDTL MEYER FUNCTION AND FLOW ANGLE IN CORE.      AXS0249
      APM = PMC(I-1,J)+PMC(I-1,J+1)+TETAC(I-1,J+1)-TETAC(I-1,J)         AXS0250
      IF (KD.EQ.2) GO TO 151                                            AXS0251
      BPM = DSIN(AMIR)*DSIN(TETAC(I-1,J+1))/RC(I-1,J+1)*DKSI            AXS0252
      CPM = DSIN(AMIL)*DSIN(TETAC(I-1,J))/RC(I-1,J)*DETA                AXS0253
  151 PMC(I,J) = (APM+BPM+CPM)/2.0                                      AXS0254
C                                                                       AXS0255
      APM = PMC(I-1,J+1)-PMC(I-1,J)+TETAC(I-1,J+1)+TETAC(I-1,J)         AXS0256
      TETAC(I,J) = (APM+BPM-CPM)/2.0                                    AXS0257
C                                                                       AXS0258
C DEFINE MACH NUMBER (BY ITERATIONS)                                    AXS0259
C INITIAL GUESS AMCOR(I,J)=AMCOR(I-1,J+1)                               AXS0260
C                                                                       AXS0261
      AMG = AMCOR(I-1,J+1)                                              AXS0262
      KZ = 0                                                            AXS0263
  154 IF (KZ.GE.100) GO TO 160                                          AXS0264
      KZ = KZ+1                                                         AXS0265
      C = AMG*AMG*A3+1.                                                 AXS0266
      D = DSQRT(AMG*AMG-1.)                                             AXS0267
      PMCAL = A2*DATAN(B2*D)-DATAN(D)                                   AXS0268
      DELNI = PMCAL - PMC(I,J)                                          AXS0269
      DEL = DABS(DELNI)                                                 AXS0270
      IF (DEL.LT..000002) GO TO 160                                     AXS0271
      IF (DELNI.LT.0.) GO TO 156                                        AXS0272
      AMG = AMG*.999                                                    AXS0273
      GO TO 154                                                         AXS0274
  156 AMG = AMG*(1.-DELNI*C/D)                                          AXS0275
      GO TO 154                                                         AXS0276
  160 AMCOR(I,J) = AMG                                                  AXS0277
C.....................................................................AXS0278
C                                                                       AXS0279
C CALCULATE FLOW PARAMETERS                                             AXS0280
      IF (J.GT.1) GO TO 197                                             AXS0281
      C = AMCOR(I,J)*AMCOR(I,J)*A3+1.                                   AXS0282
      PRES = PSTG/(C**B1)                                               AXS0283
      TEMP = TSTG/C                                                     AXS0284
      DN   = PRES/(BOLTZ*TEMP)                                          AXS0285
      FP   = .707/(DN*CXS)                                              AXS0286
      SCALE = DKSI * DSIN(ALFAL)                                        AXS0287
      AKN = FP/SCALE                                                    AXS0288
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      SOUND = DSQRT(GAMA*RJ*TEMP)                                          AXS02890
      VEL = SOUND*AMCOR(I,J)                                               AXS02900
C                                                                          AXS02910
C BREAKDOWN PARAMETER AS DEFINED BY 'BIRD'.                                AXS02920
      DENSF(I,J) = PRES/(RJ*TEMP)                                          AXS02930
      DDENS = DENSF(I-1,J) - DENSF(I,J)                                    AXS02940
      COLF  = 4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM))                         AXS02950
      P = VEL*DDENS/(SCALE*DENSF(I,J)*COLF)                                AXS02960
  197 CONTINUE                                                             AXS02970
C                                                                          AXS02980
C     TIME1 = SCALE/VEL                                                    AXS02990
C     TIME2 = 3./(4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM)))                    AXS03000
C     P = TIME2/TIME1                                                      AXS03010
C*************************************************************************AXS03020
C*************************************************************************AXS03030
C*************************************************************************AXS03040
      WRITE(6,11)I,J,AMCOR(I,J),RC(I,J),XC(I,J),TETAC(I,J),TEMP,PRES,VELAXS03050
     1,AKN,FP,DN,P                                                         AXS03060
  199 CONTINUE                                                             AXS03070
C                                                                          AXS03080
C*************************************************************************AXS03090
C*************************************************************************AXS03100
C MATCH CORE AND FAN POINTS                                                AXS03110
      DO 200 I=1,N1                                                        AXS03120
      X(I,1) =XC(I,1)                                                      AXS03130
      R(I,1)= RC(I,1)                                                      AXS03140
      AM(I,1) = AMCOR(I,1)                                                 AXS03150
      PM(I,1) = PMC(I,1)                                                   AXS03160
  200 TETA(I,1) = TETAC(I,1)                                               AXS03170
C                                                                          AXS03180
C*************************************************************************AXS03190
C*************************************************************************AXS03200
C                                                                          AXS03210
C CALCULATE FLOW PARAMETERS IN REGION 2 (SIMPLE PRANDTL MEYER FAN).        AXS03220
C                                                                          AXS03230
C*************************************************************************AXS03240
      WRITE (6,298)                                                        AXS03250
  298 FORMAT ('1','     REGION    2'/)                                     AXS03260
C                                                                          AXS03270
      KFIN = 51                                                            AXS03280
C                                                                          AXS03290
      DO 299 I = 2,N1                                                      AXS03300
      WRITE(6,10)                                                          AXS03310
      DO 299 J = 2,N2                                                      AXS03320
      IF (J.GT.KFIN) GO TO 299                                             AXS03330
      KZ = 0                                                               AXS03340
      AMIL =DARSIN(1./AM(I-1,J))                                           AXS03350
      AMIR =DARSIN(1./AM(I,J-1))                                           AXS03360
      ALFAL = PI-(TETA(I-1,J)+AMIL)                                        AXS03370
      ALFAR = TETA(I,J-1)-AMIR                                             AXS03380
C                                                                          AXS03390
C CHECK ANGLES AND CALCULATE COORDINATES                                   AXS03400
      ANGLE1 = PI/2.-.000001                                               AXS03410
      ANGLE2 = PI/2.+.000001                                               AXS03420
      IF (ALFAL.LE.ANGLE1.OR.ALFAL.GE.ANGLE2) GO TO 201                    AXS03430
      X(I,J) = X(I-1,J)                                                    AXS03440
      GO TO 207                                                            AXS03450
  201 IF (ALFAR.LE.ANGLE1.OR.ALFAR.GE.ANGLE2) GO TO 205                    AXS03460
      X(I,J) = X(I,J-1)                                                    AXS03470
      GO TO 207                                                            AXS03480
C                                                                          AXS03490
  205 X(I,J) = (R(I-1,J)-R(I,J-1)+X(I,J-1)*DTAN(ALFAR)+X(I-1,J)*DTAN(ALFAXS03500
     1AL))/(DTAN(ALFAL)+DTAN(ALFAR))                                       AXS03510
C                                                                          AXS03520
  207 IF (ALFAL.LE.0.000001.OR.ALFAL.GE.0.000001) GO TO 209                AXS03530
      R(I,J) = R(I-1,J)                                                    AXS03540
      GO TO 213                                                            AXS03550
  209 IF (ALFAR.LE.0.000001.OR.ALFAR.GE.0.000001) GO TO 211                AXS03560
      R(I,J) = R(I,J-1)                                                    AXS03570
      GO TO 213                                                            AXS03580
C                                                                          AXS03590
  211 R(I,J) = (X(I,J)-X(I,J-1))*DTAN(ALFAR)+R(I,J-1)                      AXS03600
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  213 DKSI = DSQRT((R(I,J)-R(I,J-1))**2+(X(I,J)-X(I,J-1))**2)          AXS03610
      DETA = DSQRT((R(I,J)-R(I-1,J))**2+(X(I,J)-X(I-1,J))**2)          AXS03620
C                                                                      AXS03630
      IF (R(I,J).GT.0..AND.X(I,J).GT.0.) GO TO 219                     AXS03640
      KFIN = J-1                                                       AXS03650
      WRITE(6,12)                                                      AXS03660
   12 FORMAT(' ',' FURTHER POINTS ON THE CHARACTERISTICS ARE DIVERGENT')AXS03670
  219 CONTINUE                                                         AXS03680
C LOCATION OF THE NEW MESH POINT HAS BEEN FOUND                        AXS03690
C                                                                      AXS03700
C                                                                      AXS03710
C CALCULATE NOW PRANDTL MEYER FUNCTION AND FLOW DIRECTION FOR NEW POINT AXS03720
      APM = PM(I,J-1)+PM(I-1,J)-TETA(I-1,J)+TETA(I,J-1)                AXS03730
      IF (KD.EQ.2) GO TO 251                                           AXS03740
      BPM = DSIN(AMIR)*DSIN(TETA(I,J-1))/R(I,J-1)*DKSI                 AXS03750
      CPM = DSIN(AMIL)*DSIN(TETA(I-1,J))/R(I-1,J)*DETA                 AXS03760
  251 PM(I,J) = .5*(APM+BPM+CPM)                                       AXS03770
C                                                                      AXS03780
      APM = PM(I,J-1)-PM(I-1,J)+TETA(I,J-1)+TETA(I-1,J)                AXS03790
      TETA(I,J) = .5*(APM+BPM-CPM)                                     AXS03800
C                                                                      AXS03810
C CALCULATE NOW MACH NUMBER FOR EACH POINT                             AXS03820
C INITIAL GUESS AM(I,J) = AM(I-1,J)                                    AXS03830
      AMG = AM(I-1,J)                                                  AXS03840
      KZ = 0                                                           AXS03850
  254 IF (AMG.GT.200.) GO TO 257                                       AXS03860
      D = DSQRT(AMG*AMG-1.)                                            AXS03870
      GO TO 258                                                        AXS03880
  257 D = AMG                                                          AXS03890
  258 IF (KZ.GE.100) GO TO 260                                         AXS03900
      KZ = KZ + 1                                                      AXS03910
      PMCAL = A2*DATAN(B2*D)-DATAN(D)                                  AXS03920
      DELNI = PMCAL - PM(I,J)                                          AXS03930
      DEL = DABS(DELNI)                                                AXS03940
      IF (DEL.LT..000002) GO TO 260                                    AXS03950
      IF (DELNI.LT.0.)GO TO 256                                        AXS03960
      AMG = AMG*.999                                                   AXS03970
      GO TO 254                                                        AXS03980
C////////////////////////////////////////////////////////////////////// AXS03990
  256 IF (AMG.LT.2000.)GO TO 2560                                      AXS04000
      KFIN = J-1                                                       AXS04010
      GO TO 299                                                        AXS04020
C//////////////////////////////////////////////////////////////////////AXS04030
 2560 D1 = (A3*AMG*AMG+1.)                                             AXS04040
      AMG = AMG*(1.-DELNI*D1/D)                                        AXS04050
      GO TO 254                                                        AXS04060
C                                                                      AXS04070
  260 AM(I,J) = AMG                                                    AXS04080
C CALCULATE NOW LOCAL TEMPERATURE,PRESSURE,VELOCITY,KNUDSEN NO.        AXS04090
      C = AM(I,J)*AM(I,J)*A3+1                                         AXS04100
      PRES = PSTG/(C**B1)                                              AXS04110
      TEMP = TSTG/C                                                    AXS04120
      DN = PRES/(BOLTZ*TEMP)                                           AXS04130
      DENSF(I,J) = PRES/(RJ*TEMP)                                      AXS04140
      DDENS = DENSF(I-1,J-1)-DENSF(I,J)                                AXS04150
      SCALE = DSQRT((X(I,J)-X(I-1,J-1))**2+(R(I,J)-R(I-1,J-1))**2)     AXS04160
C**************************************                                AXS04170
C                                                                      AXS04180
  271 FP = .707/(DN*CXS)                                               AXS04190
C                                                                      AXS04200
      AKN = FP/SCALE                                                   AXS04210
      SOUND =DSQRT(GAMA*RJ*TEMP)                                       AXS04220
      VEL = AM(I,J)*SOUND                                              AXS04230
C                                                                      AXS04240
C                                                                      AXS04250
      COLF = 4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM))                      AXS04260
      P = VEL*DDENS/(SCALE*DENSF(I,J)*COLF)                            AXS04270
C                                                                      AXS04280
C PRINT RESULTS FOR MESH POINTS                                        AXS04290
      KL = (-1)**I                                                     AXS04300
      IF (KL.LT.0) GO TO 299                                           AXS04310
      WRITE(6,11)I,J,AM(I,J),R(I,J),X(I,J),TETA(I,J),TEMP,PRES,VEL,AKN, AXS04320
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     1FP,DN,P                                                                  AXS04330
  299 CONTINUE                                                                 AXS04340
C                                                                              AXS04350
C*****************************************************************************AXS04360
C*****************************************************************************AXS04370
C                                                                              AXS04380
C MATCH 'REGION 2' AND 'REGION 3' POINTS                                       AXS04390
C                                                                              AXS04400
C*****************************************************************************AXS04410
      L = KFIN- 1                                                              AXS04420
      DO 300 J = 1,L                                                           AXS04430
      XX(1,J)    = X(20,J)                                                     AXS04440
      RX(1,J)    = R(20,J)                                                     AXS04450
      AMX(1,J)   = AM(20,J)                                                    AXS04460
      PMX(1,J)   = PM(20,J)                                                    AXS04470
  300 TETAX(1,J) = TETA(20,J)                                                  AXS04480
C*****************************************************************************AXS04490
C*****************************************************************************AXS04500
C                                                                              AXS04510
C CACULATE FLOW PARAMETERS FOR REGION 3                                        AXS04520
C                                                                              AXS04530
C*****************************************************************************AXS04540
      WRITE (6,397)                                                            AXS04550
  397 FORMAT ('1','   REGION    3'/)                                           AXS04560
      DO 399 I = 2,L                                                           AXS04570
      DO 399 J = I,L                                                           AXS04580
      IF (J.GT.KFIN) GO TO 399                                                 AXS04590
      IF (J.GT.I)GO TO 320                                                     AXS04600
      WRITE (6,10)                                                             AXS04610
  320 KZ = 0                                                                   AXS04620
C                                                                              AXS04630
      AMIL = DARSIN(1./AMX(I-1,J))                                             AXS04640
      ALFAL = PI-(TETAX(I-1,J)+AMIL)                                           AXS04650
      IF (J.GT.I) GO TO 301                                                    AXS04660
      ALFAR = ALFAL                                                            AXS04670
      TETAX(I,J) = PI*.5                                                       AXS04680
      TETAX(I,J-1) = PI-TETAX(I-1,J)                                           AXS04690
      XX(I,J) = 0.                                                             AXS04700
      RX(I,J) = RX(I-1,J)+XX(I-1,J)*DTAN(ALFAL)                                AXS04710
      RX(I,J-1) = RX(I-1,J)                                                    AXS04720
      XX(I,J-1) = -XX(I-1,J)                                                   AXS04730
      DKSI = (RX(I,J)-RX(I-1,J))/DSIN(ALFAL)                                   AXS04740
      DETA = DKSI                                                              AXS04750
      PMX(I,J-1) = PMX(I-1,J)                                                  AXS04760
      GO TO 316                                                                AXS04770
  301 AMIR = DARSIN(1./AMX(I,J-1))                                             AXS04780
      ALFAR = TETAX(I,J-1)-AMIR                                                AXS04790
C                                                                              AXS04800
      IF (ALFAL.LE.ANGLE1.OR.ALFAL.GE.ANGLE2) GO TO 302                        AXS04810
      XX(I,J) = XX(I-1,J)                                                      AXS04820
      GO TO 307                                                                AXS04830
  302 IF(ALFAR.LE.ANGLE1.OR.ALFAR.GE.ANGLE2) GO TO 305                         AXS04840
      XX(I,J) = XX(I,J-1)                                                      AXS04850
      GO TO 307                                                                AXS04860
  305 XX(I,J) = (RX(I-1,J)-RX(I,J-1)+XX(I,J-1)*DTAN(ALFAR)+XX(I-1,J)*DTAAXS04870
     1N(ALFAL))/(DTAN(ALFAL)+DTAN(ALFAR))                                      AXS04880
C                                                                              AXS04890
  307 IF (ALFAL.LE.0.000001.OR.ALFAL.GE.0.000001) GO TO 309                    AXS04900
      RX(I,J) = RX(I-1,J)                                                      AXS04910
      GO TO 315                                                                AXS04920
  309 IF (ALFAR.LE.0.000001.OR.ALFAR.GE.0.000001) GO TO 311                    AXS04930
      RX(I,J) = RX(I,J-1)                                                      AXS04940
      GO TO 315                                                                AXS04950
  311 RX(I,J) = RX(I,J-1)+(XX(I,J)-XX(I,J-1))*DTAN(ALFAR)                      AXS04960
C                                                                              AXS04970
  315 DKSI = DSQRT((RX(I,J)-RX(I,J-1))**2+(XX(I,J)-XX(I,J-1))**2)              AXS04980
      DETA = DSQRT((RX(I,J)-RX(I-1,J))**2+(XX(I,J)-XX(I-1,J))**2)              AXS04990
  316 CONTINUE                                                                 AXS05000
C                                                                              AXS05010
      IF (RX(I,J).GE.0..AND.XX(I,J).GE.0.)GO TO 319                            AXS05020
      KFIN = J-1                                                               AXS05030
      WRITE (6,398)                                                            AXS05040
```

```
  398 FORMAT (' ','FURTHER POINTS ON THE CHARACTERISTICS ARE DIVERGENT')AXS0505
C                                                                       AXS0506
C LOCATION OF THE NEW POINT HAS BEEN FOUND                              AXS0507
C***********************************************************************AXS0508
C                                                                       AXS0509
C CALCULATE NOW P.M. ANGLE AND FLOW DIRECTION                           AXS0510
  319 APM = PMX(I,J-1)+PMX(I-1,J)-TETAX(I-1,J)+TETAX(I,J-1)             AXS0511
      IF(KD.EQ.2) GO TO 351                                             AXS0512
      BPM = DSIN(AMIR)*DSIN(TETAX(I,J-1))/RX(I,J-1)*DKSI                AXS0513
      CPM = DSIN(AMIL)*DSIN(TETAX(I-1,J))/RX(I-1,J)*DETA                AXS0514
  351 PMX(I,J) = .5*(APM+BPM+CPM)                                       AXS0515
      APM = PMX(I,J-1)-PMX(I-1,J)+TETAX(I,J-1)+TETAX(I-1,J)             AXS0516
      TETAX(I,J) = .5*(APM+BPM+CPM)                                     AXS0517
C                                                                       AXS0518
C CALCULATE NOW THE MACH NUMBER FOR EACH POINT                          AXS0519
C INITIAL GUESS AMX(I,J) = AMX(I-1,J)                                   AXS0520
      AMG = AMX(I-1,J)                                                  AXS0521
      KZ = 0                                                            AXS0522
      KH=0                                                              AXS0523
      KL=0                                                              AXS0524
  354 IF (AMG.GT.2000.) GO TO 357                                       AXS0525
      D = DSQRT(AMG*AMG-1.)                                             AXS0526
      GO TO 358                                                         AXS0527
  357 D = AMG                                                           AXS0528
  358 IF (KZ.GE.50)GO TO 360                                            AXS0529
      KZ = KZ +1                                                        AXS0530
      PMCAL = A2*DATAN(B2*D)-DATAN(D)                                   AXS0531
      DELNI = PMCAL-PMX(I,J)                                            AXS0532
      DEL = DABS(DELNI)                                                 AXS0533
      IF (DEL.LT..000002) GO TO 360                                     AXS0534
      IF (DELNI.LT.0.)GO TO 356                                         AXS0535
      AMG = AMG*.98                                                     AXS0536
      GO TO 354                                                         AXS0537
  356 IF (AMG.LT.5000.) GO TO 3560                                      AXS0538
      KFIN = J-1                                                        AXS0539
      GO TO 399                                                         AXS0540
 3560 D1 = A3*AMG*AMG+1.                                                AXS0541
C*****************************                                        AXS0542
      DDELNI = DELNI                                                    AXS0543
      IF (AMG.GT.20.) DDELNI = DELNI*(.95**KZ)                          AXS0544
C*****************************                                        AXS0545
      AMG = AMG*(1.-DDELNI*D1/D)                                        AXS0546
      GO TO 354                                                         AXS0547
  360 AMX(I,J) = AMG                                                    AXS0548
C                                                                       AXS0549
C CALCULATE NOW THE LOCAL TEMPERATURE, PRESSURE, VELOCITY,KNUDSEN       AXS0550
      C = AMX(I,J)*AMX(I,J)*A3+1.                                       AXS0551
      PRES = PSTG/(C**B1)                                               AXS0552
      TEMP = TSTG/C                                                     AXS0553
      DN = PRES/(BOLTZ*TEMP)                                            AXS0554
C*****************************************************************     AXS0555
      DENSF(I,J)=PRES/(RJ*TEMP)                                         AXS0556
      DDENS=DENSF(I-1,J-1)-DENSF(I,J)                                   AXS0557
      FP = .707/(DN*CXS)                                                AXS0558
      SCALE=DSQRT((XX(I,J)-XX(I-1,J-1))**2+(RX(I,J)-RX(I-1,J-1))**2)    AXS0559
      AKN=FP/SCALE                                                      AXS0560
C                                                                       AXS0561
C                                                                       AXS0562
C*****************************************************************     AXS0563
C     ALFALL = -ALFAL+PI                                                AXS0564
C     AF = ALFALL-PI/2.                                                 AXS0565
C     AF = DABS(AF)                                                     AXS0566
C     IF (AF.LT..000001) GO TO 370                                      AXS0567
C     BF = 1./DSQRT(1. + DTAN(ALFALL)**2)                               AXS0568
C     SCALE=BF*(RX(I,J-1)-DTAN(ALFALL)*(XX(I,J-1)-XX(I-1,J))-RX(I-1,J)) AXS0569
C     SCALE = DABS(SCALE)                                               AXS0570
C*****************************************************************     AXS0571
      SOUND = DSQRT(GAMA*RJ*TEMP)                                       AXS0572
      VEL = AMX(I,J)*SOUND                                              AXS0573
C                                                                       AXS0574
      COLF=4.*CXS*DN*DSQRT(BOLTZ*TEMP/(PI*GMM))                         AXS0575
      P=VEL*DDENS/(SCALE*DENSF(I,J)*COLF)                               AXS0576
```

```
C                                                                       AXS05770
C PRINT RESULTS                                                         AXS05780
      WRITE(6, 11)I,J,AMX(I,J),RX(I,J),XX(I,J),TETAX(I,J),TEMP,PRES,VEL,AXS05790
     1AKN,FP,DN,P                                                       AXS05800
  399 CONTINUE                                                          AXS05810
      STOP                                                              AXS05820
      END                                                               AXS05830
$ENTRY                                                                  AXS05840
```

A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM'.

Parameter Name	Physical Name	Units	Type	Description
PAMB	ambient pressure	pascals	real	ambient atmosphere pressure
KD	K dimensions	-	integer	KD=2 for two dimensional jet KD=3 for axisymmetric ring jet
PI	π	-	real constant	
BOLTZ	Boltzmann constant	$\frac{\text{Joule}}{\text{degree}}$	real	1.38032 10^{-23} joules/degree
AVOG	Avogadro's constant	$\frac{\text{molecules}}{\text{mol}}$	real	6.0225 x 10^{26} 1/kmol
RG	Universal gas constant	$\frac{\text{Joule}}{\text{mol.deg}}$	real	8314.3
AM0	Mach No. (E.P)	-	real	Mach number at exit plane
T0	Temperature (E.P)	°k	real	Temperature at exist plane
P0	Pressure (E.P)	pascals	real	Pressure at exit plane
R1	Cylinder radius	m	real	Radius of the cylindrical vehicle
X1	0.5* nozzle width	m	real	Half width of nozzle
GAMA		-	real	averaged heat capacity ratio (jet)
DIAM	Molecule diameter	m	real	averaged molecular diameter (jet)
GM	Molecular mass	kg/kmol	real	averaged molecular weight (jet)
RJ	Gas constant	$\frac{\text{joules}}{\text{kj.deg}}$	real	gas constant (jet)
CXS		m^2	real	collision cross section (hard sphere)
GMM	mass of a molecule	kg	real	averaged mass of a molecule
N1			integer	number of divisions (characteristics from the exist plane)
N2			integer	number of characteristics in the Prandtl Meyer fan
A1			real	$\frac{\gamma - 1}{\gamma}$
B1			real	$\frac{\gamma}{\gamma - 1}$

A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM' (CONTINUED)

Parameter Name	Physical Name	Units	Type	Description
A2			real	$[(\gamma + 1)/(\gamma - 1)]$
B2			real	1/A2
A3			real	$\frac{\gamma - 1}{2}$
C			real	$M^2 \frac{\gamma - 1}{2} + 1$
D,D1,D2			real	$M^2 - 1$
PSTG		pascals	real	stagnation pressure
TSTG		°k	real	stagnation temperature
DSTG		kg/m^3	real	stagnation density
FSM			real	free stream Mach number
FST		°k	real	free stream temperature
FSD		kg/m^3	real	free stream density
AMIT	μ_T	radius	real	Mach angle (tail of P.M. fan)
AMIH	μ_H	radius	real	Mach angle (head of P.M. fan)
PMT	ν_T	radius	real	P.M. function (tail)
PMH	ν_H	radius	real	P.M. function (head)
RAT,RAT2, E1			real	used to define a loparithmic division of the corner characteristics (50 lines in P.M. fan)(a linear division would have resulted in concentration of characteristics at high Mach numbers)
DELM			real	difference of Mach numbers
AM(I,J)	M		real 2-D array	Mach number at location (I,j)(used for the corner)
PM(I,J)	ν	radius		P.M. function at location (I,j)(used for the corner)
AMI	μ	radius	real	Mach angle
R(I,J)		m	real 2-D array	radius (or ordinate) at (I,j)
TETA(I,J)	θ	radius	real 2-D array	flow direction at (I,j)

A.4 LIST OF MAIN SYMBOLS USED IN 'AXSYM' (CONTINUED)

Parameter Name	Physical Name	Units	Type	Description
ALFAL		radians	real	angle of a left running characteristics
ALFAR		radians	real	angle of a right running characteristics
DENSF(I,J)		k_g/m^3	real 2-D array	gas density at point IJ
AMCOR(I,J)			real 2-D array	Mach number at mesh points in region (1) (region 1 is bounded by the two tail characteristics
TETAC(I,J)		radians	real 2-D array	flow direction at mesh points (region 1)
PMC(I,J)		radians	real 2-D array	P.M. function at mesh points (region 1)
XC(I,J)		m	real 2-D array	X coordinate at mesh points (region 1)
RC(I,J)		m	real 2-D array	radius (ordinate) at mesh points (region 1)
AMIL		radians	real	Mach angle far left running characteristics
AMIR		radians	real	Mach angle far right running characteristics
DKSI	$d\xi$	m	real	distance between mesh points
DETA	$d\eta$	m	real	distance between mesh points
DELNI	$d\nu$	radians	real	P.M. differential
AMG		radians		Mach number (used for iterative calculation)
PRES				pressure
TEMP				temperature
DN				number density
FP				mean free path
AKN				Knudsen number
SOUND				speed of sound
VEL				absolute local velocity
DDENS				density difference between two points along a steamline
COLF				collision frequency
P				breakdown parameter

A.5 AXSYM PROGRAM USER'S GUIDE

1. Input data:

ambient pressure	PAMB
Mach number (Exit plane)	AMO
Temperature (Exit plane)	TO
Pressure (Exit plane)	PO
Half width of nozzle	X1
Radius of nozzle ring	R1
Specific heat ratio of jet gas	GAMA
average molecular diameter (jet)	DIAM
average molecular weight	GM

2. Options for flow geometry

two dimensional flow	KD=2
ring jet	KD=3
default condition	KD=3

3. Resolution of mesh points

   to change the resolution of the mesh points

   a - change N1 and N2 as necessary

   b - change 'DIMENSIONS' according to new values of N_1 and N2

   c - define distribution of Mach lines in the Prandtl-Meyer fan as required (program lines 126-131)

4. Execution commands:

   After copying program into USER'S FILE:

   WATFIV AXSYM * (XTYPE

   The program will run on user's terminal under WATFIV. A soft copy of program listing and output listing will be stored in user's disk named AXSYM LISTING.

5. Hard Copy

PRINT AXSYM LISTING.

6. Program Outputs.

All necessary outputs are automatically listed by the program.

Figure (20) and Figure (21) show the resulting mesh of characteristics calculated for an altitude of 200 km for MO=4 and MO=2 respectively.

In these figures we also show some isotherms and the limit where the breakdown parameter equals 0.05. These lines are plotted (manually) using interpolation procedures. Data along the breakdown line is input data for the molecular flow.

APPENDIX B SIMUL PROGRAM

B.1 DATA ORGANIZATION

Because of the large number of molecules, cells, regions and sectors in the simulation and the large number of data related to each molecule, each cell and region to be stored, special precautions should be taken in order not to overflow the available computer memory.

The following data organization was used in SIMUL. Figure 22 shows the geometry of one sector.

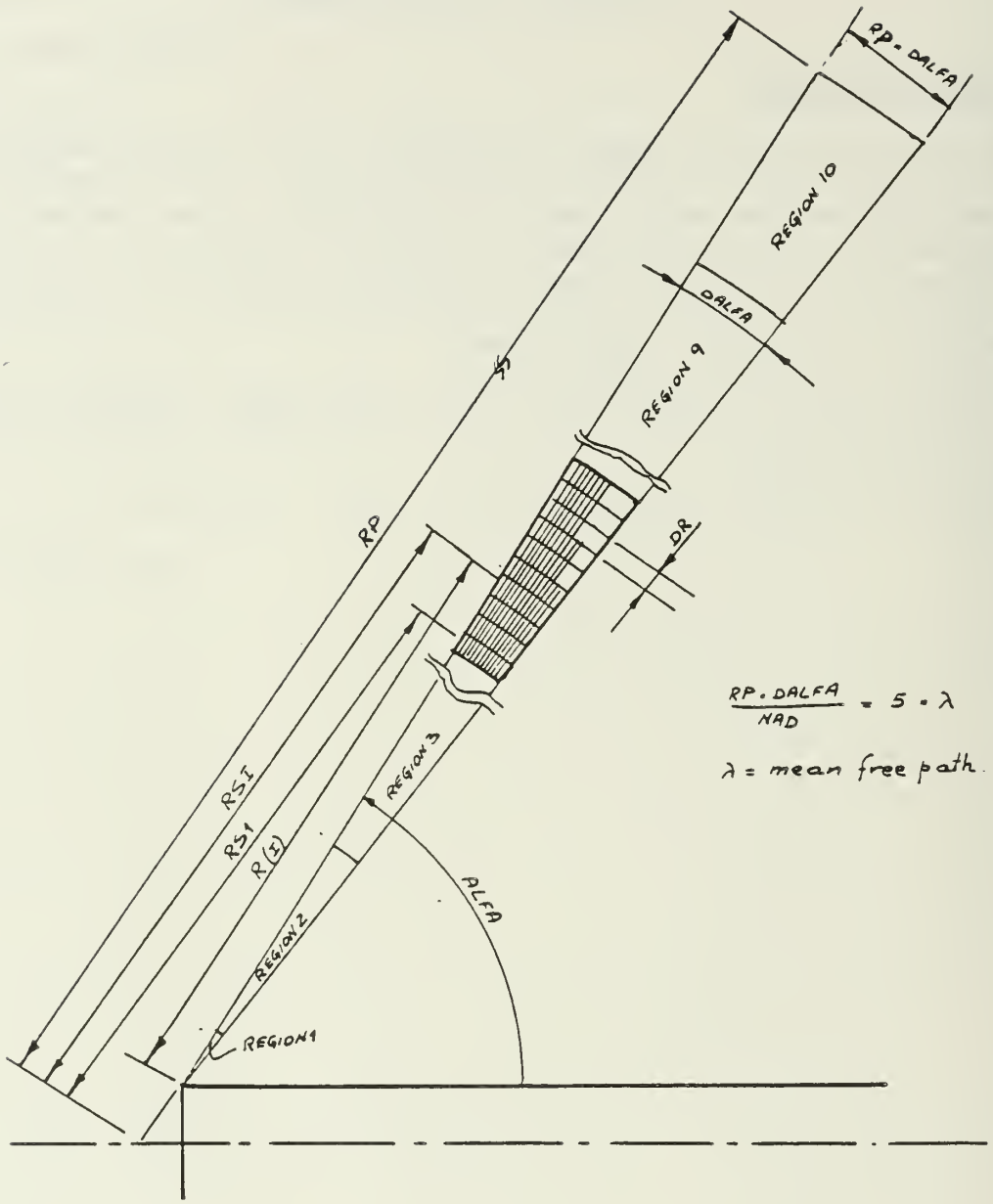

Figure 22. Definition of sector geometry and cell volume.

cell volume = v(I) = R(I) * DDALFA x DR x RSI * DFI.

$$\frac{v(I)}{v(1)} = \frac{R(I) \cdot RSI(I)}{R(1) \cdot RSI}$$

v(1) is the volume of smallest cell in a region.

1. Tables of Molecules and Their Parameters

P1(L,N1M) - Light molecules of the jet

P2(L,N2M) - Heavy molecules of the jet

P3(L,N3M) - Ambient gas molecules (not used in the present program)

N1M, N2M, N3M - maximum number of molecules in simulation. Number of active molecules may be smaller or equal to (N<I>M).

L=1,2,3 - cartesian components of velocity v_x, v_y, v_z [m/s]

L=4 - radial coordinate [meters]

if r=-99 the particular molecule is inactive

L=5 - angular coordinate [radians].

This table is generated each time the simulation is initiated for a region. That means, the same group of molecules (as stored in the computer memory) is used to simulate the flow in all regions in the computation domain.

2. C(M,I,j) Table of Cells (in a Region)-Real Data

I = 1,10 - radial index of the cell in a region

j = 1,10 - angular index of the cell in a region

M = 19 - radial coordinate of cell center

M = 20 - angular coordinate of cell center

M = 1,9 - time parameter for collisions of different species in a cell

M = 10-18 - maximum relative velocity expected for collisions of different species in a cell

3. IP(N1A+N2A+N3A) Table of the addresses of the active molecules arranged in order of their species and in the order of their cells

IC(N,I,j) - table of cells (in a region) integer data

I = 1,10 - radial index

j = 1,10 - angular index

N = 1 - number of molecules (spec 1)

N = 2 - number of molecules (spec 2)

N = 3 - number of molecules (spec 3)

N = 4 - (starting address - 1) of molecules as ordered in (IP).

4. Reg(N,kR,kS) Data table for a specific region (real)

kR = 1,10 - index of a region in a sector

kS = 1,20 - index of the sector

N = 1 - Df1 = differential angle (axisymmetric)

DF1 is a weighting factor

N = 2 - DN1 = number density (species 1)

N = 3 - DN2 = number density (species 1)

N = 4 - VOL 1 = actual volume of smallest cell in kR

N = 5 - AREA1 INPUT area of smallest cell in kR

5. Region Geometry and Input Flux

R(10) - polar radius of a cell in a region

A(10) - $\frac{\text{input area of a cell}}{\text{input area of smallest cell}}$

VOL(10) - $\frac{\text{volume of a cell}}{\text{volume of smallest cell}}$

M1(10) - initial number of molecules in cells

(equal number of molecules of either jet species)

F1(10),F2(10) - input flux through high pressure starting line

(spec 1), (spec 2)

6. Input Flux From High Pressure Starting Line

FWP1(N,I,j)

FWP2(N,I,j)

```
↑↑↑↑
|||species
|||
||positive (input molecules)
||
|west
|
flux
```

I = 1,10 - number of the cell along the starting line in a region (j)

j = 1,10 - number of the region along the starting line

N = 1 - molecular flow for a given DF1

N = 2 - mean molecular velocity Vx

N = 3 - mean molecular velocity Vy

N = 4 - mean input gas temperature

7. Output Flux

FNN1(4,NAD,kR) FSN1(4,NAD,kR)

FNN2(4,NAD,kR) FSN2(4,NAD,kR)

```
↑↑                      ↑↑
|negative (output)       |negative (output)
|                        |
north                    south
```

kR - number of region in the sector

NAD - angular location

The first index include the same parameters as (FWP1)

FEN1(4,NRD) FWN1(4,NRD)

FEN2(4,NRD) FWN2(4,NRD)

```
↑↑                      ↑↑
|negative               |negative
|                       |
east                    west
```

NRD → radial location

FEN1,FEN2,FWN1,FWN2 are necessary for iterations within one sector.

8. Sampling of Output Flux from a Sector

After averaging they are transferred to FOE1, FOE2, FOW1, FOW2.

FOW1(4,kC,kR,kS)
FOW2(4,kC,kR,kS) — output flow to the west

FOE1(4,kC,kR,kS)
FOE2(4,kC,kR,kS) — output flow to the east

kC - radial location (cell) of flow in a region

kR - index of a region in a sector

kS - index of the sector

The first index (4 parameters) include the same parameters as FEP1( ).

B.2 MOLECULAR SIMULATION FOR A GIVEN REGION

After we define the geometry of the whole sector resulting from the region geometry and cell geometry, we may start with the molecular simulation. This includes:

- initial setting of molecules in cells
- molecules are moved according to the time increment DTM
- new molecules are generated according to input (or output) flows
- collisions calculations
- integration of flow parameters for average parameters calculations
- repetition of the whole procedure as long as necessary to obtain reasonable statistical averaging
- calculate averages and flow weighting.

These routines are the core of the program and must be repeated for all regions in a sector and (or all sectors in the domain where the collisions are significant).

In the following sections we bring a detailed description of this part of the program.

1. Initial Setting of Molecules in Cells

   a. The initial number of available molecules in a simulation is larger than the number of active molecules (P1(data, number of molecules), P2(data, number of molecules) are the vectors used for species 1 and 2)

   b. an inactive molecule is defined as

$$[P1(4,N) \text{ or } P2(4,N)] = -99$$

c. calculation of number of molecules to be set in each cell

d. calculation of cell coordinates

e. deactivation of all available molecules in simulation

f. definition of molecules coordinates

P1(4,N), P2(4,M) are polar radiuses

P1(5,N), P2(5,M) are angular coordinate in radians

All molecules in a cell are set at random locations within the cell.

g. definition of molecular velocities

P1(1,N), P2(1,M) velocity in X direction

P1(2,N), P2(2,M) velocity in Y direction

P1(3,N), P2(3,M) velocity in Z direction

Thermal velocities are random function of temperatures and are added to the mean velocity as defined at initial boundary $ALFA_o$ of the region.

As the thermal velocity has a Boltzmann distribution the thermal velocity setting is based on rejection-acceptance methods (for more details see Bird [4] Appendix D).

h. reset collision timers and relative velocity

i. reset general time counter: Time = 0

3. The Simulation

a. Move all molecules according to their velocity (V_x, V_y) and find their new coordinates

Note - A routine designed to calculate the collisions with the wall was included in the program; if the region (or sector) is bounded by the solid wall, the collision is calculated - resulting new velocities and directions and counted for wall flux calculations. If the program is stopped at an angle where the flow becomes collisionless, this routine becomes irrelevant and other type of calculations should be designed.

b. Output flow counting: all molecules that leave the region are counted and stored in specific vectors which are used as inputs to other regions. The output vectors are (X represent 1 or 2 for the two species in the program (FSNX))

FSNX(1,j,kR) → "south" boundary

FNNX(1,j,kR) → "north" boundary

FENX(1,I) → "east" boundary

FWNX(1,I) → "west" boundary

I represents the radial location index of the cell

j represents the angular location index

kR is the index of the region within a sector

Note - all molecules that move to

(j=NAD+1)(I=NRD+1) are placed in FENX(1,NRD)

(j= -1)(X=NRD+1) are placed in FWNX(1,NRD)

(j=NAD+1)(I= -1) are placed in FSNX(1,1,kR)

(j= -1)(I= -1) are placed in FWNX(1,1,kR)

This was done only for simplification reasons.

c. Generation of new molecules due to input flows. Through the four sides E,N,W,S, of a region, molecules are allowed to enter the region according with the flows coming from the neighbouring regions:

for "W" side of the region in sector 1

FWPX(P,I,kR)

for other sectors

FOEX(P,I,kR,kS-1)

for "E" side of any region

FOWX(P,I,kR,kS+1)

for "N" side of any region

FSNX(P,j,kR+1)

for "S" side of the region

FNNX(P,j,kR-1)

The first parameter of all these arrays represent:

P = 1 - number flux (real number)

P = 2 - velocity component - (V_x)

P = 3 - velocity component - (V_y)

P = 4 - gas temperature

Note 1 - because every region has a different size of angle DFI, all fluxes have to be adjusted accordingly.

Note 2 - input fluxes are calculated, adjusted and stored as real numbers. The number of input molecules are by definition integers. In order not to "loose" molecules, the number of input molecules is increased by 1 on a random basis. (The average of many runs will result in the accurate average input flow.)

New molecules are set at random locations on the boundary of the specific cells and at random time within DTM. Then each molecule is allowed to enter the region according to its initial coordinate and velocity. At the end of the time interval the new location and velocity is stored in molecule array P1 or P2. If DTM is chosen to be too large and cell size is small (total region size too small) some molecules may cross the region and will not be counted in the simulation of the specific region. In order not to "loose" molecules:

(a) DTM should be decreased

(b) count these molecules as output fluxes from the specific region. (This is recommended only if there is no other choice.)

Note - Because the arrays of input flows store only averaged data for the molecules, the thermal velocity of each new molecule is calculated according to the Boltzmann distribution as a function of the averaged temperature.

d. Rearrangement of molecules in cells. Before collisions are calculated all simulated molecules which have been let to move and generated have to be rearranged and recounted for each cell.

The array IC(k,I,j) contains integer data for each cell (I,j)

k = 1 - is the number of molecules of species 1

k = 2 - is the number of molecules of species 2

k = 3 - is the number of molecules of species 3 (not used)

k = 4 - is the (address-1) of the first molecule in the cell related to the vector IP(M)

Vector IP(M) contains the list of the simulated molecules arranged in the order of species in cells and cells respectively. The following is a graphic description of IP(M)

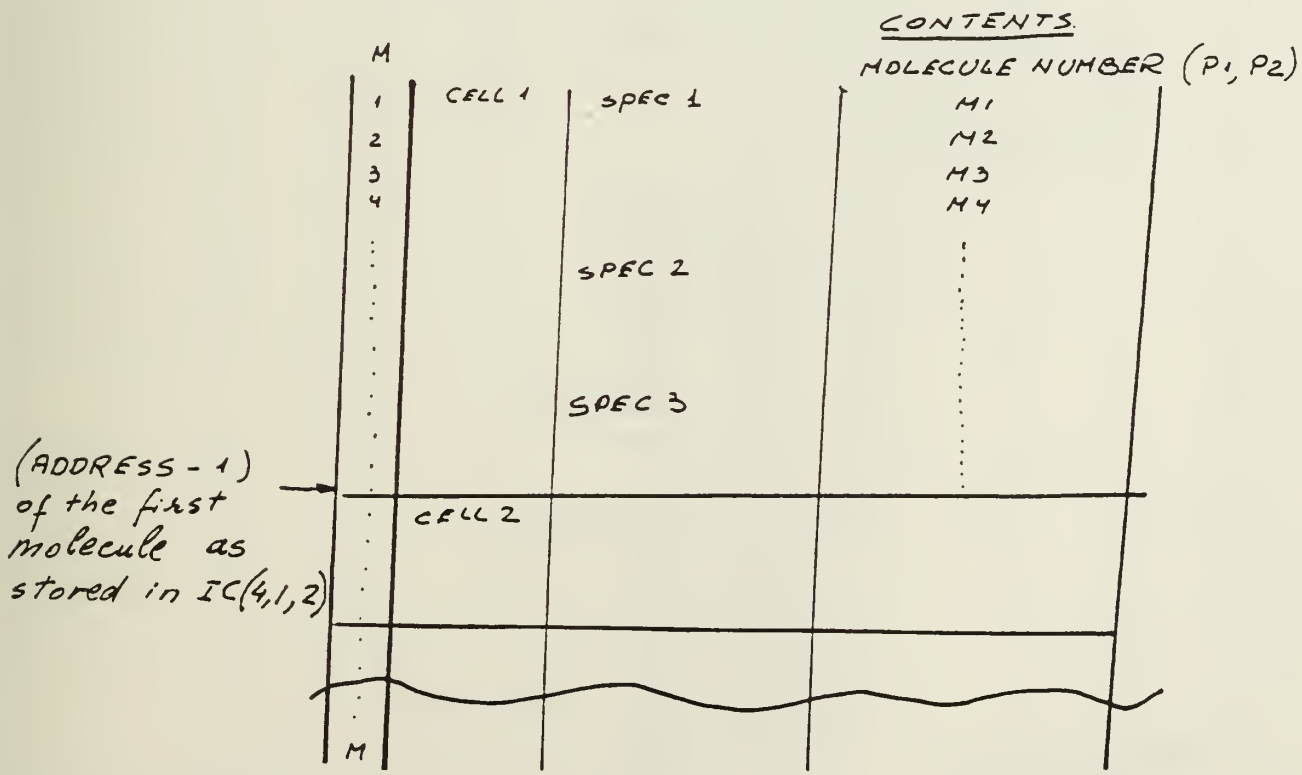

Figure 23. Vector IP(M)

B.3 SIMUL Program Flowchart

A simplified flowchart for the Monte Carlo simulation of the molecular flow is shown in Figure 24. The program is designed to solve the ring axisymmetric jet flow, however, minor changes may be done to enable a different geometry.

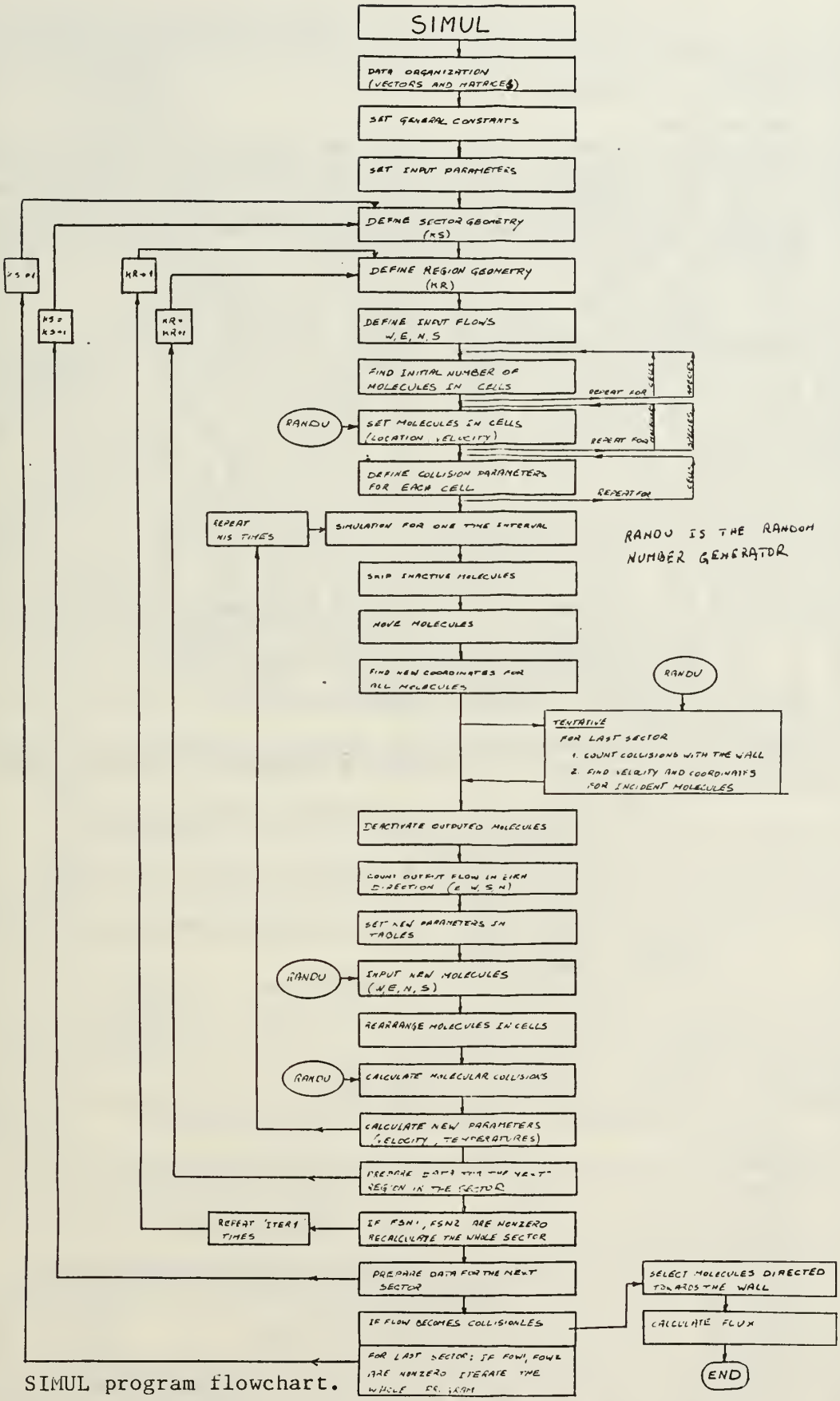

Figure 24. SIMUL program flowchart.

B.4 SIMUL Program Listing

```
C     PROGRAM SIMUL                                                     SIM00010
C THIS PROGRAM IS DESIGNED TO CALCULATE THE MOLECULAR FLOW OUTSIDE THE  SIM00020
C CONTINUUM REGION FLOW OF A HIGHLY UNDEREXPANDED AXISYMMETRIC RING JET.SIM00030
C RESULTS FOR THE CONTINUUM FLOW MAY BE OBTAINED FROM 'AXSYM' PROGRAM   SIM00040
C WHICH GIVES THE 'METHOD OF CHARACTERISTICS' ISENTROPIC SOLUTION.      SIM00050
C THE BOUNDARY BETWEEN THE CONTINUUM AND MOLECULAR FLOW IS DEFINED BY   SIM00060
C THE BREAKDOWN PARAMETER 'P' AS PROPOSED BY G. A. BIRD.                SIM00070
C THE 'MOLECULAR DOMAIN' IS DIVIDED INTO POLAR DIVISIONS MAKING A SET   SIM00080
C OF SECTORS. EACH SECTOR IS SUDIVIDED INTO 10 REGIONS                  SIM00090
C NO APRIORY INFORMATION ABOUT THE GEOMETRY OF THE DIFFERENT            SIM00100
C REGIONS IS AVAILABLE, THEREFORE, MANUAL INTERVENTION MAY BE           SIM00110
C REQUIRED WHEN MOVING FROM ONE SECTOR TO THE OTHER. AN ACCEPTABLE      SIM00120
C GEOMETRY WILL RESULT A REASONABLE NUMBER OF SIMULATED MOLECULES.      SIM00130
C EACH REGION IS SUBDIVIDED INTO A NUMBER OF CELLS WITH A GEOMETRY      SIM00140
C DEFINED BY A POLAR MESH. A NUMBER OF MOLECULES IS SET IN EACH CELL    SIM00150
C PROPORTIONAL TO THE CELL VOLUME. THE BOUNDARY CONDITIONS FOR EACH     SIM00160
C REGION REQUIRE INPUT AND OUTPUT FLUX OF MOLECULES. NO APRIORY         SIM00170
C INFORMATION ON THE FLUX IS AVAILABLE. IT WILL BE CALCULATED IN        SIM00180
C AN ITERATIVE MODE.                                                    SIM00190
C IF THE BOUNDARY CONDITIONS FOR ALL CELLS ARE CONSTANT THE NUMBER      SIM00200
C FLUX INTO EACH CELL IS PROPORTIONAL TO CELL WALL AREA.                 SIM00210
C TO DECREASE THE ERROR WHEN INTRODUCING MOLECULES -(INTEGER NUMBER)-   SIM00220
C DUE TO THE INPUT FLUX -(REAL NUMBER), AN ADDITIONAL MOLECULE IS       SIM00230
C GENERATED ON THE BASIS OF RANDOM NUMBERS SUCH THAT THE AVERAGE OF A   SIM00240
C LARGE NUMBER OF SAMPLINGS WILL EQUAL THE REAL INPUT FLUX.             SIM00250
C*********************************************************************** SIM00260
C          THE MONTE CARLO SIMULATION                                   SIM00270
C THE JET GAS IS COMPOSED OF TWO SPECIES OF MOLECULES                   SIM00280
C AMBIENT GAS IS REGARDED AS ONE SPECIES                                SIM00290
C THE MOLECULAR MODEL IS - 'HARD SPHERE MOLECULE'                       SIM00300
C NETWORK DEFINITION                                                    SIM00310
C    THE MAXIMUM RADIUS (POLAR) OF THE DOMAIN IS ASSUMED TO BE RP=15 M. SIM00320
C    THE ANGLE OF THE BOUNDARY BETWEEN CONTINUUM AND MOLECULAR FLOW     SIM00330
C    AND THE SOLID WALL IS                                              SIM00340
C                ALFA  (CALCULATED IN PROGRAM 'AXSYM')                  SIM00350
C    DEFINE A POLAR SECTOR WITH A RADIUS 'RP' AND AN ANGLE OF           SIM00360
C                DALFA =5*MFP*NAD/RP                                    SIM00370
C    THIS SECTOR IS SUBDIVIDED INTO A NUMBER OF RADIAL DIVISIONS        SIM00380
C    MAKING 'N' REGIONS FOR SIMULATION CALCULATIONS FOR EACH 'DALFA'.   SIM00390
C    EACH REGION IS DEVIDED INTO                                        SIM00400
C         NAD -ANGULAR DIVISIONS (15) WITH AN ANGLE OF DDALFA=5*MFP/RP  SIM00410
C         NRD -RADIAL  DIVISIONS (10)                                   SIM00420
C             MAKING NAD*NRD CELLS                                      SIM00430
C    THE SMALLEST CELL CONTAINS 'MIN' MOLECULES                         SIM00440
C                    MIN = 15                                           SIM00450
C    TOTAL NUMBER OF ACTIVE MOLECULES IN A REGION IS LIMITED TO 6000    SIM00460
C    (3000 MOLECULES OF EACH SPECIES.)                                  SIM00470
C THE WIDTH OF A CELL DEFINED BY ANGLE 'DFI' MAY NOW BE EVALUATED.      SIM00480
C (MIN/NUMBER DENSITY = ACTUAL CELL VOLUME)                             SIM00490
C*********************************************************************SIM00500
C        DEFINE PARAMETERS.....................................BLOCK 1SIM00510
      COMMON IX                                                         SIM00520
      DIMENSION P1(5,3000),P2(5,3000),IP(6000),C(20,10,15),             SIM00530
     *IC(4,10,15),REG(5,10,20)                                          SIM00540
C     DIMENSION DFI(10),DN(10)                                          SIM00550
      DIMENSION R(10),A(10),VOL(10),M1(10),F1(10),F2(10)                SIM00560
      DIMENSION SS(2,10,10)                                             SIM00570
      DIMENSION FEN1(4,10),FWN1(4,10),FNN1(4,15,10),FSN1(4,15,10)       SIM00580
      DIMENSION FEN2(4,10),FWN2(4,10),FNN2(4,15,10),FSN2(4,15,10)       SIM00590
      DIMENSION FWP1(4,10,10),FWP2(4,10,10)                             SIM00600
      DIMENSION FOE1(4,10,10,20),FOW1(4,10,10,20)                       SIM00610
      DIMENSION FOE2(4,10,10,20),FOW2(4,10,10,20)                       SIM00620
      DIMENSION NM(3),VRC(3),TOC(3,3),SPEC(3,5),NCOL(10,15)             SIM00630
C P1,P2,P3 CONTAIN INFORMATION ON UP TO M SIMULATED MOLECULES           SIM00640
C   P1(1,N),P1(2,N),P1(3,N) ARE U,V,W VELOCITY COMPONENTS (CARTESIAN)   SIM00650
C   P1(4,N),P1(5,N) ARE R AND TETA COORDINATES (POLAR)                  SIM00660
C                                                                       SIM00670
C IP(M) ARE THE M MOLECULES ARRANGED IN THE ORDER OF THEIR CELLS        SIM00680
C C(20,I,J) CONTAINS INFORMATION ON UP TO I*J CELLS                     SIM00690
C*********************************************************************SIM00700
C                                                                       SIM00710
C ALFA IS THE ANGLE WHERE THE BREAKDOWN PARAMETER EQUALS .05   .        SIM00720
```

```
C FPM IS THE MEAN FREE PATH AT ALFA.                                    SIM00730
C*************************************************************************SIM00740
C SET GENERAL CONSTANTS.....................................BLOCK 2SIM00750
      IX     = 529814367                                                SIM00760
      PI     = 3.141593                                                 SIM00770
      BOLTZ  = 1.38044E-23                                              SIM00780
      P0     = 101325.                                                  SIM00790
      T0     = 273.                                                     SIM00800
      AVOG   = 2.68699E+25                                              SIM00810
      RG     = 8314.                                                    SIM00820
C*************************************************************************SIM00830
C SET PROGRAM CONSTANTS.....................................BLOCK 3SIM00840
      ISPEC=2                                                           SIM00850
      R1 = 2.5                                                          SIM00860
      DR=.15                                                            SIM00870
      RP=15.                                                            SIM00880
C NUMBER OF SIMULATED MOLECULES IN SMALLEST CELL (DIFFERENT SPECIES)    SIM00890
      NMOL1=3000                                                        SIM00900
      NMOL2=3000                                                        SIM00910
      NMOL3=0                                                           SIM00920
      MIN = 15                                                          SIM00930
      N1M = 15                                                          SIM00940
      N2M = 15                                                          SIM00950
C NUMBER OF DIVISIONS IN A SIMULATED REGION                             SIM00960
      NAD = 15                                                          SIM00970
      NRDS=10                                                           SIM00980
      NRD=10                                                            SIM00990
      NRD1= 3                                                           SIM01000
      NIS =2                                                            SIM01010
C R1 IS THE RADIUS OF THE CYLINDER (WALL)                               SIM01020
C R(I) IS THE RADIAL COORDINATE OF CELL(I)                              SIM01030
C VOL(I) IS THE RATIO BETWEEN VOLUMES OF CELL(I) AND CELL(1)            SIM01040
C A(I) IS THE RATIO BETWEEN INPUT FLOW AREAS OF CELL(I) AND CELL(1)     SIM01050
C DR IS THE RADIAL SIZE OF A CELL (RADIAL INCREMENT)                    SIM01060
C INPUT THE FOLLOWING AS 'DATA' OR 'READ' STATEMENTS ****************   SIM01070
      TETA = 1.2                                                        SIM01080
C TETA IS THE FLOW DIRECTION (RADIANS) ON THE BREAKDOWN LINE AS FOUND   SIM01090
C FROM THE AXSYM PROGRAM. V0 IS THE FLOW VELOCITY (M/SEC)               SIM01100
      V0   = 2100                                                       SIM01110
      V0X  = V0*COS(TETA)                                               SIM01120
      V0Y  = V0*SIN(TETA)                                               SIM01130
      TWALL=300.                                                        SIM01140
      DN01=1.1E21                                                       SIM01150
      DN02=1.1E21                                                       SIM01160
      DTM=1.5E-6                                                        SIM01170
C SET DATA FOR THE DIFFERENT SPECIES                                    SIM01180
C   MOLECULAR MASS                                                      SIM01190
      SPEC(1,1)=4./AVOG                                                 SIM01200
      SPEC(2,1)=40./AVOG                                                SIM01210
      SPEC(3,1)=29./AVOG                                                SIM01220
C   MOLECULAR DIAMETER                                                  SIM01230
      SPEC(1,2)=2.19E-10                                                SIM01240
      SPEC(2,2)=4.00E-10                                                SIM01250
C     SPEC(3,2)=                                                        SIM01260
C     SPEC(1,3)=                                                        SIM01270
C     SPEC(2,3)=     ADDITIONAL DATA IF REQUIRED                        SIM01280
C     SPEC(3,3)=                                                        SIM01290
C*************************************************************************SIM01300
C THERMAL VELOCITIES AT WALL TEMPERATURE                                SIM01310
      VWM1=SQRT(2.*BOLTZ*TWALL/SPEC(1,1))                               SIM01320
      VWM2=SQRT(2.*BOLTZ*TWALL/SPEC(2,1))                               SIM01330
C                                                                       SIM01340
C*************************************************************************SIM01350
C INITIALISATION..RESET ALL SAMPLING VARIABLES                          SIM01360
      DO 80 I=1,NRD                                                     SIM01370
      DO 80 JR=1,10                                                     SIM01380
      DO 80 JS=1,20                                                     SIM01390
      DO 80 KPAR=1,4                                                    SIM01400
      FOE1(KPAR,I,JR,JS)=0.                                             SIM01410
      FOE2(KPAR,I,JR,JS)=0.                                             SIM01420
      FOW1(KPAR,I,JR,JS)=0.                                             SIM01430
   80 FOW2(KPAR,I,JR,JS)=0.                                             SIM01440
```

```
C*************************************************************************SIM01450
C SET INPUT PARAMETERS.....................................BLOCK 3 SIM01460
      ITER=1                                                            SIM01470
C RETURN TO 3000 FOR ADDITIONAL ITERATIONS                              SIM01480
 3000 KS=1                                                              SIM01490
      ALFA=1.3                                                          SIM01500
      FPM=.001                                                          SIM01510
      TEMP=40.                                                          SIM01520
      VTER1=SQRT(2.*BOLTZ*TEMP/SPEC(1,1))                               SIM01530
      VTER2=SQRT(2.*BOLTZ*TEMP/SPEC(2,1))                               SIM01540
      IF (ITER.GT.1)GO TO 2005                                          SIM01550
      DO 2001 I=1,10                                                    SIM01560
      REG(2,I,1)=DN01                                                   SIM01570
      REG(3,I,1)=DN02                                                   SIM01580
      DO 2001 J=1,10                                                    SIM01590
      FWP1(2,I,J)=V0X                                                   SIM01600
      FWP2(2,I,J)=V0X                                                   SIM01610
      FWP1(3,I,J)=V0Y                                                   SIM01620
      FWP2(3,I,J)=V0Y                                                   SIM01630
      FWP1(4,I,J)=TEMP                                                  SIM01640
 2001 FWP2(4,I,J)=TEMP                                                  SIM01650
 2005 CONTINUE                                                          SIM01660
C                                                                       SIM01670
C*************************************************************************SIM01680
C                                                                       SIM01690
C*************************************************************************SIM01700
C DEFINE SECTOR GEOMETRY...................................BLOCK 4 SIM01710
C KR IS THE INDEX FOR A REGION IN ONE SECTOR                            SIM01720
C RETURN TO 1000 FOR NEXT SECTOR                                        SIM01730
      DALFA=0.                                                          SIM01740
 1000 KR=1                                                              SIM01750
C RESET SAMPLING OF FLOW VARIABLES    (N AND S)                         SIM01760
      DO 81 I=1,NAD                                                     SIM01770
      DO 81 JR=1,10                                                     SIM01780
      DO 81 KPAR=1,4                                                    SIM01790
      FNN1(KPAR,I,JR)=0.                                                SIM01800
      FNN2(KPAR,I,JR)=0.                                                SIM01810
      FSN1(KPAR,I,JR)=0.                                                SIM01820
   81 FSN2(KPAR,I,JR)=0.                                                SIM01830
C ALFA IS THE STARTING ANGLE OF THE PRESENT SECTOR. PREVIOUS DALFA      SIM01840
C SUBTRACTED FROM PREVIOUS ALFA (PREVIOUS SECTOR) GIVES THE NEW ALFA.   SIM01850
      ALFA=ALFA-DALFA                                                   SIM01860
      DALFA = 5.*FPM*FLOAT(NAD)/RP                                      SIM01870
C DALFA IS THE ANGLE OF THE SECTOR                                      SIM01880
      IF(DALFA.GT.ALFA/2.)DALFA=ALFA/2.                                 SIM01890
      IF(DALFA.GT.(FPM*75/RP))DALFA=ALFA                                SIM01900
      IF(ALFA.LE.0.)GO TO 2000                                          SIM01910
      DDALFA = DALFA/FLOAT(NAD)                                         SIM01920
C DDALFA IS THE ANGLE OF A SINGLE CELL IN THE SECTOR                    SIM01930
      ALFAJ=ALFA-DALFA/2.                                               SIM01940
C                                                                       SIM01950
C*************************************************************************SIM01960
C DEFINE REGION KR IN SECTOR...............................BLOCK 5 SIM01970
C RETURN TO 2000 FOR THE NEXT REGION KR                                 SIM01980
 2000 CONTINUE                                                          SIM01990
C RESET SAMPLING OF FLOW VARIABLES PER REGION                           SIM02000
      DO 82 I=1,NRD                                                     SIM02010
      DO 82 KPAR=1,4                                                    SIM02020
      FEN1(KPAR,I)=0.                                                   SIM02030
      FEN2(KPAR,I)=0.                                                   SIM02040
      FWN1(KPAR,I)=0.                                                   SIM02050
   82 FWN2(KPAR,I)=0.                                                   SIM02060
      MT=0                                                              SIM02070
      NRD=NRDS                                                          SIM02080
      IF(KR.LT.2)NRD=NRD1                                               SIM02090
      DO 100 I = 1,NRD                                                  SIM02100
C POLAR RADIUS MEASURED FROM THE NOZZLE LIP                             SIM02110
      R(I) =(FLOAT(I)-.5)*DR                                            SIM02120
      IF(KR.EQ.2)R(I)=R(I)+FLOAT(NRD1)*DR                               SIM02130
      IF(KR.GE.3)R(I)=R(I)+(FLOAT(NRD1+(KR-2)*NRD))*DR                  SIM02140
C RSI IS THE RADIUS MEASURED FROM THE AXIS OF SYMMETRY                  SIM02150
      RSI=R(I)+R1/SIN(ALFAJ)                                            SIM02160
```

```
      IF(I.EQ.1)RS1=RSI                                                 SIM02170
      A(I)   = RSI/RS1                                                  SIM02180
      VOL(I) = R(I)*RSI/(R(1)*RS1)                                      SIM02190
      M1(I)  = MIN*VOL(I)                                               SIM02200
      MT = MT+M1(I)                                                     SIM02210
C M1() IS THE INITIAL NUMBER OF MOLECULES IN EACH CELL                  SIM02220
      DN1=REG(2,KR,KS)                                                  SIM02230
      DN2=REG(3,KR,KS)                                                  SIM02240
      REG(1,KR,KS)=FLOAT(MIN)/(DN1*R(1)*RS1*DR*DDALFA)                  SIM02250
C DFI (REG(1,KR,KS)) IS THE SPHERICAL (AXISYMMETRIC) ANGLE              SIM02260
C THIS ANGLE HAS DIFFERENT VALUES FOR EACH KR, THEREFORE IT IS A        SIM02270
C WEIGHTING FACTOR.+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+=+  SIM02280
C  (FNN1,FNN2,FSN1,FSN2,FEN1,FEN2,FWN1,FWN2) *   DFI                  SIM02290
C  (FOE1,FOE2,FOW1,FOW2)                     *   DFI                  SIM02300
      DA1 = RS1*DR*REG(1,KR,KS)                                         SIM02310
C DA1 IS THE INPUT AREA OF CELL(1)                                      SIM02320
      FN1 = V0*DA1*REG(2,KR,KS)*SIN(ALFA-TETA)                          SIM02330
      FN2 = V0*DA1*REG(3,KR,KS)*SIN(ALFA-TETA)                          SIM02340
C TETA IS THE ANGLE BETWEEN FLOW DIRECTION AND THE WALL                 SIM02350
      F1(I) = FN1*A(I)                                                  SIM02360
      F2(I) = FN2*A(I)                                                  SIM02370
C                                                                       SIM02380
   99 FWP1(1,I,KR)=F1(I)                                                SIM02390
  100 FWP2(1,I,KR)=F2(I)                                                SIM02400
C.....                                                                  SIM02410
C DEFINE ACTUAL VOLUME AND INPUT AREA OF SMALLEST CELL IN REGION        SIM02420
      REG(4,KR,KS)=R(1)*DDALFA*DR*RS1*REG(1,KR,KS)                      SIM02430
      REG(5,KR,KS)=DA1                                                  SIM02440
C FN1 IS THE NUMBER FLUX TO THE SMALLEST CELL (REAL NUMBER) PER SECOND. SIM02450
C INPUT NUMBER OF MOLECULES (INTEGER) WILL BE INTEGRATED TO MAKE AN     SIM02460
C AVERAGE OF FN1.                                                       SIM02470
C F1(I) IS THE INPUT FLUX TO CELL(I)                                    SIM02480
C  FOLLOWING ARE THE REGION BOUNDARIES                                  SIM02490
  102 RMIN=R(1)-.5*DR                                                   SIM02500
      RMAX=RMIN+DR*FLOAT(NRD)                                           SIM02510
      TMAX=ALFA                                                         SIM02520
      TMIN=ALFA-DALFA                                                   SIM02530
      DO 9102 I = 1,NRD                                                 SIM02540
      WRITE (6,9101)R(I),A(I),VOL(I),M1(I),F1(I)                        SIM02550
9101  FORMAT(' ',3F13.5,I10,E15.5)                                      SIM02560
9102  CONTINUE                                                          SIM02570
      MTT= MT*NAD                                                       SIM02580
      WRITE(6,103)MT,MTT                                                SIM02590
  103 FORMAT (' INITIAL NUMBER OF SIMULATED MOLECULES IS= ',I5,' PER SPESIM02600
     XCIES PER DDALFA, TOTAL NUMBER IS', I5)                            SIM02610
C*********************************************************************SIM02620
C DEFINE INPUT FLOWS TO KR W,E,N,S.............................BLOCK 6 SIM02630
C                                                                       SIM02640
C                                                                       SIM02650
C                                                                       SIM02660
C*********************************************************************SIM02670
C CALCULATE INITIAL NUMBER OF MOLECULES IN CELLS................BLOCK 7 SIM02680
C SET INITIAL STATE OF GAS.....................................  ''  8 SIM02690
C                                                                       SIM02700
      DO 150 I =1,NRD                                                   SIM02710
      DO 150 J= 1,NAD                                                   SIM02720
C                                                                       SIM02730
C SET SIMULATED MOLECULES IN THEIR CELLS                                SIM02740
      IC(1,I,J) = M1(I)                                                 SIM02750
      IC(2,I,J) = M1(I)                                                 SIM02760
      IC(3,I,J) = 0                                                     SIM02770
C                                                                       SIM02780
C SET CELL COORDINATES                                                  SIM02790
      C(19,I,J) = R(I)                                                  SIM02800
      C(20,I,J) = ALFA-(FLOAT(J)-.5)*DDALFA                             SIM02810
  150 CONTINUE                                                          SIM02820
C*********************************************************************SIM02830
C                                                                       SIM02840
C DEACTIVATE ALL MOLECULES                                              SIM02850
      DO 170 N = 1,NMOL1                                                SIM02860
      P1(4,N) = -99.                                                    SIM02870
  170 P2(4,N) = -99.                                                    SIM02880
```

```
C                                                                       SIM02890
C*********************************************************************** SIM02900
C SET INITIAL STATE OF THE GAS (LOCATION AND VELOCITY OF MOLECULES)      SIM02910
C                                                                       SIM02920
      NADR1 = 0                                                         SIM02930
      NADR2 = 0                                                         SIM02940
      DO 200 I = 1,NRD                                                  SIM02950
      DO 200 J = 1,NAD                                                  SIM02960
      NM1 = IC(1,I,J)                                                   SIM02970
C                                                                       SIM02980
      DO 205 N = 1,NM1                                                  SIM02990
      NADR1 = NADR1 + 1                                                 SIM03000
      CALL RANDU(PP)                                                    SIM03010
      P1(4,NADR1) = C(19,I,J)+DR*(PP-.5)                                SIM03020
      CALL RANDU(P)                                                     SIM03030
      P1(5,NADR1) = C(20,I,J)+DDALFA*(P-.5)                             SIM03040
C                                                                       SIM03050
      DO 205 NV = 1,3                                                   SIM03060
  203 CALL RANDU(P)                                                     SIM03070
      V = -3.+6.*P                                                      SIM03080
      B = EXP(-V*V)                                                     SIM03090
      CALL RANDU(P)                                                     SIM03100
      IF(B.LT.P) GO TO 203                                              SIM03110
      P1(NV,NADR1) = P*SIN(B)*VTER1                                     SIM03120
      IF(NV.EQ.1)P1(NV,NADR1)=P1(NV,NADR1)+V0X                          SIM03130
      IF(NV.EQ.2)P1(NV,NADR1)=P1(NV,NADR1)+V0Y                          SIM03140
  205 CONTINUE                                                          SIM03150
C                                                                       SIM03160
C REPEAT PROCEDURE FOR SPECIES 2                                        SIM03170
      NM2 =IC(2,I,J)                                                    SIM03180
      DO 210 N = 1,NM2                                                  SIM03190
      NADR2 = NADR2+1                                                   SIM03200
      CALL RANDU(P)                                                     SIM03210
      P2(4,NADR2) = C(19,I,J)+DR*(P-.5)                                 SIM03220
      CALL RANDU(P)                                                     SIM03230
      P2(5,NADR2) = C(20,I,J)+DDALFA*(P-.5)                             SIM03240
C                                                                       SIM03250
      DO 210 NV = 1,3                                                   SIM03260
  207 CALL RANDU(P)                                                     SIM03270
      V = -3.+6.*P                                                      SIM03280
      B = EXP(-V*V)                                                     SIM03290
      CALL RANDU(P)                                                     SIM03300
      IF(B.LT.P) GO TO 207                                              SIM03310
      P2(NV,NADR2) = P*SIN(B)*VTER2                                     SIM03320
      IF(NV.EQ.1)P2(NV,NADR2)=P2(NV,NADR2)+V0X                          SIM03330
      IF(NV.EQ.2)P2(NV,NADR2)=P2(NV,NADR2)+V0Y                          SIM03340
  210 CONTINUE                                                          SIM03350
C                                                                       SIM03360
C WHEN NECESSARY, REPEAT PROCEDURE FOR SPECIES 3.                       SIM03370
  200 CONTINUE                                                          SIM03380
C                                                                       SIM03390
C*********************************************************************** SIM03400
C DEFINE HERE ALL COLLISION PARAMETERS TO BE INCLUDED IN SIMULATION      SIM03410
C                                                                BLOCK 9 SIM03420
C RESET COLLISION TIMERS                                                SIM03430
      DO 19 I=1,NRD                                                     SIM03440
      DO 19 J=1,NAD                                                     SIM03450
      DO 19 L=1,3                                                       SIM03460
      DO 19M=1,3                                                        SIM03470
      KT=3*(L-1)+M+9                                                    SIM03480
      C(KT,I,J)=0.                                                      SIM03490
C SET EXPECTED MAXIMUM RELATIVE VELOCITY IN COLLISIONS                  SIM03500
      KV=3*(L-1)+M                                                      SIM03510
      EM1=SPEC(L,1)                                                     SIM03520
      EM2=SPEC(M,1)                                                     SIM03530
      EMR=EM1*EM2/(EM1+EM2)                                             SIM03540
C                                                                       SIM03550
      IF(KS.EQ.1)GO TO 17                                               SIM03560
      TEM=FOE1(4,I,KR,KS)                                               SIM03570
      GO TO 18                                                          SIM03580
   17 TEM=FWP1(4,I,KR)                                                  SIM03590
C                                                                       SIM03600
```

```
   18 RV=2./SQRT(PI*2.*BOLTZ*TEM/EMR)                                    SIM03610
   19 C(KV,I,J)=2.*RV                                                    SIM03620
C                                                                        SIM03630
C MAXIMUM RELATIVE VELOCITY WILL BE RESET IF FASTER ENCOUNTERS OCCUR     SIM03640
C                                                                        SIM03650
C*************************************************************************SIM03660
      TIME=0.                                                            SIM03670
C LOOP OVER TIME INTERVALS.....................................BLOCK 10   SIM03680
      DO 6000 JDTM = 1,NIS                                               SIM03690
C                                                                        SIM03700
C                                                                        SIM03710
      TIME=TIME+DTM                                                      SIM03720
C*************************************************************************SIM03730
C                                                                        SIM03740
C MOVE ALL MOLECULES ..........................................BLOCK 12   SIM03750
C MOVE MOLECULES OF SPECIES 1                                            SIM03760
C                                                                        SIM03770
      DO 310 I1 = 1,NMOL1                                                SIM03780
C SKIP INACTIVE MOLECULES.....................................13          SIM03790
      IF (P1(4,I1).EQ.-99.) GO TO 310                                    SIM03800
      VX = P1(1,I1)                                                      SIM03810
      VY = P1(2,I1)                                                      SIM03820
      RX = P1(4,I1)                                                      SIM03830
      T = P1(5,I1)                                                       SIM03840
      TOLD=T                                                             SIM03850
C*************************************************************************SIM03860
C FIND NEW COORDINATES.....................................BLOCK 14       SIM03870
      XX=RX*COS(T)+VX*DTM                                                SIM03880
      YY=RX*SIN(T)+VY*DTM                                                SIM03890
      RNEW=SQRT(XX**2+YY**2)                                             SIM03900
      T=ATAN(YY/XX)                                                      SIM03910
C*************************************************************************SIM03920
C FOR LAST SECTOR FIND COLLISIONS WITH THE WALL AND SAMPLE THEM          SIM03930
C                              .........................BLOCK 15,16       SIM03940
      IF(ALFA.GT.DALFA)GO TO 301                                         SIM03950
      IF(T.GT.0.)GO TO 301                                               SIM03960
      DTR=DTM*T/(T-TOLD)                                                 SIM03970
C DTR IS THE TIME REMAINING AFTER A MOLECULE STRIKES THE WALL            SIM03980
      IF(DTR.LT.1E-10)DTR=1E-10                                          SIM03990
      RW=RX+(RNEW-RX)*DTR/DTM                                            SIM04000
      IF(RW.LT.RMIN)RW=RMIN+DTR*.001                                     SIM04010
      IF(RW.GT.RMAX)RW=RMAX-DTR*.001                                     SIM04020
      LOC=RW/DR+1.                                                       SIM04030
C                                                                        SIM04040
C COUNT COLLISIONS WITH THE WALL(MUST BE WAIGHTED =*DFI)                 SIM04050
      SS(1,LOC,JSAMP)=SS(1,LOC,JSAMP)+1                                  SIM04060
C                                                                        SIM04070
C SET VELOCITY AND LOCATION AFTER A MOLECULE STRIKES THE WALL            SIM04080
  302 CALL RANDU(P)                                                      SIM04090
      B=VWM1*SQRT(-ALOG(P))                                              SIM04100
      CALL RANDU(P)                                                      SIM04110
      BB=2.*PI*P                                                         SIM04120
      P1(1,NADR1)=B*COS(BB)                                              SIM04130
      VX=B*COS(BB)                                                       SIM04140
      P1(2,NADR1)=B*SIN(BB)                                              SIM04150
      VY=B*SIN(BB)                                                       SIM04160
      CALL RANDU(P)                                                      SIM04170
      P1(3,NADR1)=VWM1*SQRT(-ALOG(P))                                    SIM04180
      XX=RX*COS(T)+VX*DTR                                                SIM04190
      YY=RX*SIN(T)+VY*DTR                                                SIM04200
      RNEW=SQRT(XX**2+YY**2)                                             SIM04210
      T=ATAN(YY/XX)                                                      SIM04220
C                                                                        SIM04230
C*************************************************************************SIM04240
C DEACTIVATE ALL MOLECULES THAT MOVED OUT.....................BLOCK 17   SIM04250
  301 IF(RNEW.LT.RMAX.AND.RNEW.GT.RMIN.AND.T.LT.TMAX.AND.T.GT.TMIN)GO TOSIM04260
     *303                                                                SIM04270
      RI=(RNEW-RMIN)/DR+.999999                                          SIM04280
      IR=RI                                                              SIM04290
      TI=(TMAX-T)/DDALFA+.999999                                         SIM04300
      IT=TI                                                              SIM04310
C                                                                        SIM04320
```

```
      IF(IT.LE.0)GO TO 304                                              SIM04330
      IF(IT.GT.NAD)GO TO 305                                            SIM04340
      IF(IR.GT.NRD)GO TO 306                                            SIM04350
C COUNT S DIRECTION, SAMPLE .....................................18     SIM04360
      FSN1(1,IT,KR)=FSN1(1,IT,KR)+1.                                   SIM04370
      GO TO 309                                                         SIM04380
C COUNT W DIRECTION, SAMPLE......................................18     SIM04390
  304 IF(IR.LE.0)IR=1                                                   SIM04400
      IF(IR.GT.NRD)IR=NRD                                               SIM04410
      FWN1(1,IR)=FWN1(1,IR)+1.                                          SIM04420
      GO TO 309                                                         SIM04430
C COUNT E DIRECTION, SAMPLE......................................18     SIM04440
  305 IF(IR.LE.0)IR=1                                                   SIM04450
      IF(IR.GT.NRD)IR=NRD                                               SIM04460
      FEN1(1,IR)=FEN1(1,IR)+1.                                          SIM04470
      GO TO 309                                                         SIM04480
C COUNT N DIRECTION, SAMPLE......................................18     SIM04490
  306 FNN1(1,IT,KR)=FNN1(1,IT,KR)+1.                                    SIM04500
C SET NEW VALUES IN THE MOLECULE TABLE                                  SIM04510
C                                                                       SIM04520
  309 RNEW=-99.                                                         SIM04530
  303 P1(4,I1)=RNEW                                                     SIM04540
      P1(5,I1)=T                                                        SIM04550
  310 CONTINUE                                                          SIM04560
C                                                                       SIM04570
C.....                                                                  SIM04580
C REPEAT PROCEDURE FOR SPECIES 2 MOLECULES.............BLOCKS 12 TO18   SIM04590
      DO 320 I2=1,NMOL2                                                 SIM04600
C SKIP INACTIVE MOLECULES .                                             SIM04610
      IF(P2(4,I2).EQ.-99.)GO TO 320                                     SIM04620
      VX = P2(1,I2)                                                     SIM04630
      VY = P2(2,I2)                                                     SIM04640
      RX = P2(4,I2)                                                     SIM04650
      T = P2(5,I2)                                                      SIM04660
      TOLD=T                                                            SIM04670
C                                                                       SIM04680
      XX=RX*COS(T)+VX*DTM                                               SIM04690
      YY=RX*SIN(T)+VY*DTM                                               SIM04700
      RNEW=SQRT(XX**2+YY**2)                                            SIM04710
      T=ATAN(YY/XX)                                                     SIM04720
C  COLLISIONS WITH THE WALL                                             SIM04730
C.....                                                                  SIM04740
      IF(ALFA.GT.DALFA)GO TO 311                                        SIM04750
      IF(T.GT.0.)GO TO 311                                              SIM04760
      DTR=DTM*T/(T-TOLD)                                                SIM04770
C DTR IS THE TIME REMAINING AFTER A MOLECULE STRIKES THE WALL           SIM04780
      IF(DTR.LT.1E-10)DTR=1E-10                                         SIM04790
      RW=RX+(RNEW-RX)*DTR/DTM                                           SIM04800
      IF(RW.LT.RMIN)RW=RW+DTR*.001                                      SIM04810
      IF(RW.GT.RMAX)RW=RW-DTR*.001                                      SIM04820
      LOC=RW/DR+1                                                       SIM04830
C COUNT COLLISIONS WITH THE WALL (MUST BE WEIGHTED =*DFI)               SIM04840
      SS(2,LOC,JSAMP)=SS(2,LOC,JSAMP)+1                                 SIM04850
C                                                                       SIM04860
C FIND THE NEW COORDINATES OF THE MOLECULE                              SIM04870
  312 CALL RANDU(P)                                                     SIM04880
      B=VWM2*SQRT(-ALOG(P))                                             SIM04890
      CALL RANDU(P)                                                     SIM04900
      BB=2.*PI*P                                                        SIM04910
      P2(1,NADR2)=B*COS(BB)                                             SIM04920
      VX=B*COS(BB)                                                      SIM04930
      P2(2,NADR2)=B*SIN(BB)                                             SIM04940
      VY=B*SIN(BB)                                                      SIM04950
      CALL RANDU(P)                                                     SIM04960
      XX=RX*COS(T)+VX*DTR                                               SIM04970
      YY=RX*SIN(T)+VY*DTR                                               SIM04980
      RNEW=SQRT(XX**2+YY**2)                                            SIM04990
      T=ATAN(YY/XX)                                                     SIM05000
C                                                                       SIM05010
C DEACTIVATE MOLECULES THAT MOVED OUT.COUNT FOR OUTPUT FLUX EVALUATION. SIM05020
  311 IF(RNEW.LT.RMAX.AND.RNEW.GT.RMIN.AND.T.LT.TMAX.AND.T.GT.TMIN)GO TOSIM05030
     *313                                                               SIM05040
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```
      RI = (RNEW-RMIN)/DR+.999999                                       SIM05050
      IR = RI                                                           SIM05060
      TI = (TMAX-T)/DDALFA+.999999                                      SIM05070
      IT = TI                                                           SIM05080
      IF (IT.LE.0)GO TO 314                                             SIM05090
      IF (IT.GT.NAD)GO TO 315                                           SIM05100
      IF(IR.GT.NRD)GO TO 316                                            SIM05110
C COUNT S DIRECTION, SAMPLE.....................................18       SIM05120
      FSN2(1,IT,KR)=FSN2(1,IT,KR)+1.                                    SIM05130
      GO TO 319                                                         SIM05140
C COUNT W DIRECTION, SAMPLE.....................................18       SIM05150
  314 IF(IR.LE.0)IR=1                                                   SIM05160
      IF(IR.GT.NRD)IR=NRD                                               SIM05170
      FWN2(1,IR)=FWN2(1,IR)+1.                                          SIM05180
      GO TO 319                                                         SIM05190
C COUNT E DIRECTION, SAMPLE.....................................18       SIM05200
  315 IF(IR.LE.0)IR=1                                                   SIM05210
      IF(IR.GT.NRD)IR=NRD                                               SIM05220
      FEN2(1,IR)=FEN2(1,IR)+1.                                          SIM05230
      GO TO 319                                                         SIM05240
C COUNT N DIRECTION, SAMPLE,....................................18       SIM05250
  316 FNN2(1,IT,KR)=FNN2(1,IT,KR)+1.                                    SIM05260
C                                                                       SIM05270
  319 RNEW = -99.                                                       SIM05280
C.....................................................19                SIM05290
  313 P2(4,I2)= RNEW                                                    SIM05300
      P2(5,I2)= T                                                       SIM05310
  320 CONTINUE                                                          SIM05320
C                                                                       SIM05330
C***********************************************************************SIM05340
C NOW NEW MOLECULES WILL BE INTRODUCED                                  SIM05350
C TOTAL JET FLUX INTO THE REGION WAS DETERMINED BY F1(I) MOL./SEC.      SIM05360
C OR FWP1(I,KR),FWP2(I,KR) FOR EACH SPECIES                            SIM05370
C NUMBER OF MOLECULES TO BE ACTIVATED PER DTM IS F(I)*DTM PER CELL.     SIM05380
C                                                                       SIM05390
C***********************************************************************SIM05400
      DO 390 I=1,NRD                                                    SIM05410
C INPUT 'W' MOLECULES                                                   SIM05420
      IF(KS.EQ.1)GO TO 322                                              SIM05430
      ANEW1=FOE1(1,I,KR,KS-1)                                           SIM05440
      ANEW2=FOE2(1,I,KR,KS-1)                                           SIM05450
      GO TO 323                                                         SIM05460
  322 ANEW1=FWP1(1,I,KR)*DTM                                            SIM05470
      ANEW2=FWP2(1,I,KR)*DTM                                            SIM05480
  323 NEW1=ANEW1                                                        SIM05490
      NEW2=ANEW2                                                        SIM05500
      REM1=ANEW1-NEW1                                                   SIM05510
      CALL RANDU(P)                                                     SIM05520
      IF(REM1.GT.P)NEW1=NEW1+1                                          SIM05530
      REM2=ANEW2-NEW2                                                   SIM05540
      CALL RANDU(P)                                                     SIM05550
      IF(REM2.GT.P)NEW2=NEW2+1                                          SIM05560
C ACTIVATE NEW INPUT MOLECULES                                          SIM05570
C TIME,LOCATION AND VELOCITY COMP. OF NEW MOLS. ARE RANDOM FUNCTIONS    SIM05580
C SPECIES 1.............................                                SIM05590
      IF(NEW1.LT.1)GO TO 341                                            SIM05600
C                                                                       SIM05610
      DO 340 I1=1,NEW1                                                  SIM05620
      CALL RANDU(P)                                                     SIM05630
      ATIME=P*DTM                                                       SIM05640
      CALL RANDU(P)                                                     SIM05650
      RSTART=(FLOAT(I-1)+P)*DR+RMIN                                     SIM05660
      VELX=FWP1(2,I,KR)                                                 SIM05670
      VELY=FWP1(3,I,KR)                                                 SIM05680
      TEM=FWP1(4,I,KR)                                                  SIM05690
C THERMAL VELOCITY                                                      SIM05700
      VTER1=SQRT(2.*BOLTZ*TEM/SPEC(1,1))                                SIM05710
C TEMPERATURE IS TRANSFERRED THROUGH FWP1(4,I,KR)                       SIM05720
      XX=RSTART*COS(ALFA)+VELX*ATIME                                    SIM05730
      YY=RSTART*SIN(ALFA)+VELY*ATIME                                    SIM05740
      RX=SQRT(XX**2+YY**2)                                              SIM05750
      T=ATAN(YY/XX)                                                     SIM05760
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      IF(RX.LT.RMIN.OR.RX.GT.RMAX)GO TO 340                              SIM0577
      IF(T.LT.TMIN.OR.T.GT.TMAX)GO TO 340                                SIM0578
C FOR MORE ACCURATE CALCULATION SET THESE MOLECULES IN OUTPUT FLOWS       SIM0579
C                                                                        SIM0580
C DEFINE THE VELOCITY COMPONENTS                                         SIM0581
      CALL RANDU(P)                                                      SIM0582
      B=VTER1*SQRT(-ALOG(P))                                             SIM0583
      CALL RANDU(P)                                                      SIM0584
      BB=2.*PI*P                                                         SIM0585
      VELX=VELX+B*COS(BB)                                                SIM0586
      VELY=VELY+B*SIN(BB)                                                SIM0587
      CALL RANDU(P)                                                      SIM0588
      VELZ=VTER1*SQRT(-ALOG(P))                                          SIM0589
C DEFINE THE NEW MOLECULE TO BE ACTIVATED                                SIM0590
      DO 325 IACT=1,NMOL1                                                SIM0591
      IF(P1(4,IACT).EQ.-99.)GO TO 326                                    SIM0592
  325 CONTINUE                                                           SIM0593
C                                                                        SIM0594
C IF THERE IS NO ROOM FOR ADDITIONAL MOLECULE PRINT 'ALARM'              SIM0595
      IF(IACT.GE.NMOL1)GO TO 3004                                        SIM0596
  326 P1(4,IACT)=RX                                                      SIM0597
      P1(5,IACT)=T                                                       SIM0598
      P1(1,IACT)=VELX                                                    SIM0599
      P1(2,IACT)=VELY                                                    SIM0600
      P1(3,IACT)=VELZ                                                    SIM0601
  340 CONTINUE                                                           SIM0602
C.....                                                                   SIM0603
C REPEAT PROCEDURE FOR SPECIES 2                                         SIM0604
  341 IF(NEW2.LT.1)GO TO 351                                             SIM0605
      DO 350 I2=1,NEW2                                                   SIM0606
      CALL RANDU(P)                                                      SIM0607
      ATIME=P*DTM                                                        SIM0608
      CALL RANDU(P)                                                      SIM0609
      RSTART=RMIN+(FLOAT(I-1)+P)*DR                                      SIM0610
      VELX=FWP2(2,I,KR)                                                  SIM0611
      VELY=FWP2(3,I,KR)                                                  SIM0612
      TEM=FWP2(4,I,KR)                                                   SIM0613
C THERMAL VELOCITY                                                       SIM0614
      VTER2=SQRT(2.*BOLTZ*TEM/SPEC(2,1))                                 SIM0615
      XX=RSTART*COS(ALFA)+VELX*ATIME                                     SIM0616
      YY=RSTART*SIN(ALFA)+VELY*ATIME                                     SIM0617
      RX=SQRT(XX**2+YY**2)                                               SIM0618
      T=ATAN(YY/XX)                                                      SIM0619
      IF(RX.LT.RMIN.OR.RX.GT.RMAX)GO TO 350                              SIM0620
      IF(T.LT.TMIN.OR.T.GT.TMAX)GO TO 350                                SIM0621
C FOR MORE ACCURATE RESULTS SET THESE MOLECULES IN OUTPUT FLOWS           SIM0622
C                                                                        SIM0623
C DEFINE VELOCITY COMPONENTS                                             SIM0624
      CALL RANDU(P)                                                      SIM0625
      B=VTER2*SQRT(-ALOG(P))                                             SIM0626
      CALL RANDU(P)                                                      SIM0627
      BB=2.*PI*P                                                         SIM0628
      VELX=VELX+B*COS(BB)                                                SIM0629
      VELY=VELY+B*SIN(BB)                                                SIM0630
      CALL RANDU(P)                                                      SIM0631
      VELZ=VTER2*SQRT(-ALOG(P))                                          SIM0632
C FIND A NEW MOLECULE TO BE ACTIVATED                                    SIM0633
      DO 345 IACT=1,NMOL2                                                SIM0634
      IF (P2(4,IACT).EQ.-99.)GO TO 346                                   SIM0635
  345 CONTINUE                                                           SIM0636
C IF THERE IS NO PLACE THEN PRINT ALARM                                  SIM0637
      IF(IACT.EQ.NMOL2)GO TO 3004                                        SIM0638
  346 P2(4,IACT)=RX                                                      SIM0639
      P2(5,IACT)=T                                                       SIM0640
      P2(1,IACT)=VELX                                                    SIM0641
      P2(2,IACT)=VELY                                                    SIM0642
      P2(3,IACT)=VELZ                                                    SIM0643
  350 CONTINUE                                                           SIM0644
C                                                                        SIM0645
C REPEAT PROCEDURE FOR SPEC-3                                            SIM0646
C.....SIM0647
C INPUT E MOLECULES                                                      SIM0648
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  351 IF (TMIN.LE.0.)GO TO 390                                          SIM06490
C                                                                       SIM06500
C                                                                       SIM06510
      ANEW1=FOW1(1,I,KR,KS+1)                                           SIM06520
C                                                                       SIM06530
C                                                                       SIM06540
      NEW1=ANEW1                                                        SIM06550
      REM=ANEW1-NEW1                                                    SIM06560
      CALL RANDU(P)                                                     SIM06570
      IF(P.LT.REM)NEW1=NEW1+1                                           SIM06580
C                                                                       SIM06590
      ANEW2=FOW2(1,I,KR,KS+1)                                           SIM06600
      NEW2=ANEW2                                                        SIM06610
      REM=ANEW2-NEW2                                                    SIM06620
      CALL RANDU(P)                                                     SIM06630
      IF(P.LT.REM)NEW2=NEW2+1                                           SIM06640
C                                                                       SIM06650
C                                                                       SIM06660
      IF(NEW1.LE.0)GO TO 370                                            SIM06670
C                                                                       SIM06680
      DO 362 I1=1,NEW1                                                  SIM06690
      CALL RANDU(P)                                                     SIM06700
      T=TMIN+DDALFA*P                                                   SIM06710
      CALL RANDU(P)                                                     SIM06720
      RNEW=RMIN+(FLOAT(I-1)+P)*DR                                       SIM06730
      CALL RANDU(P)                                                     SIM06740
      TEM=FOW1(4,I,KR,KS+1)                                             SIM06750
      VTER1=SQRT(2.*BOLTZ*TEM/SPEC(1,1))                                SIM06760
      B=VTER1*SQRT(-ALOG(P))                                            SIM06770
      CALL RANDU(P)                                                     SIM06780
      BB=2.*PI*P                                                        SIM06790
      VELX=FOW1(2,I,KR,KS+1)+B*COS(BB)                                  SIM06800
      VELY=FOW1(3,I,KR,KS+1)+B*SIN(BB)                                  SIM06810
      CALL RANDU(P)                                                     SIM06820
      VELZ=VTER1*SQRT(-ALOG(P))                                         SIM06830
C FIND A NEW MOLECULE TO BE ACTIVATED                                   SIM06840
      DO 364 IACT=1,NMOL1                                               SIM06850
      IF(P1(4,IACT).EQ.-99.)GO TO 366                                   SIM06860
  364 CONTINUE                                                          SIM06870
C IF THERE IS NO ROOM FOR ADDITIONAL MOLECULE THEN PRINT 'ALARM'        SIM06880
      IF(IACT.EQ.NMOL1)GO TO 3004                                       SIM06890
  366 P1(4,IACT)=RNEW                                                   SIM06900
      P1(5,IACT)=T                                                      SIM06910
      P1(1,IACT)=VELX                                                   SIM06920
      P1(2,IACT)=VELY                                                   SIM06930
  362 P1(3,IACT)=VELZ                                                   SIM06940
  370 CONTINUE                                                          SIM06950
C                                                                       SIM06960
C REPEAT FOR SPECIES 2                                                  SIM06970
      IF(NEW2.LE.0)GO TO 390                                            SIM06980
      DO 382 I2=1,NEW2                                                  SIM06990
      CALL RANDU(P)                                                     SIM07000
      T=TMIN+DDALFA*P                                                   SIM07010
      CALL RANDU(P)                                                     SIM07020
      RNEW=RMIN+(FLOAT(I-1)+P)*DR                                       SIM07030
      CALL RANDU(P)                                                     SIM07040
      TEM=FOW2(4,I,KR,KS+1)                                             SIM07050
      VTER2=SQRT(2.*BOLTZ*TEM/SPEC(2,1))                                SIM07060
      B=VTER2*SQRT(-ALOG(P))                                            SIM07070
      CALL RANDU(P)                                                     SIM07080
      BB=2.*PI*P                                                        SIM07090
      VELX=FOW2(2,I,KR,KS+1)+B*COS(BB)                                  SIM07100
      VELY=FOW2(3,I,KR,KS+1)+B*COS(BB)                                  SIM07110
      CALL RANDU(P)                                                     SIM07120
      VELZ=VTER2*SQRT(-ALOG(P))                                         SIM07130
C FIND A NEW MOLECULE TO BE ACTIVATED                                   SIM07140
      DO 384 IACT=1,NMOL2                                               SIM07150
      IF(P2(4,IACT).EQ.-99)GO TO 386                                    SIM07160
  384 CONTINUE                                                          SIM07170
C IF THERE IS NO ROOM FOR ADDITIONAL MOLECULE THEN PRINT ALARM          SIM07180
      IF(IACT.EQ.NMOL2) GO TO 3004                                      SIM07190
  386 P2(4,IACT)=RNEW                                                   SIM07200
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      P2(5,IACT)=T                                                      SIM07210
      P2(1,IACT)=VELX                                                   SIM07220
      P2(2,IACT)=VELY                                                   SIM07230
  382 P2(3,IACT)=VELZ                                                   SIM07240
C..................................................................... SIM07250
C REPEAT FOR SPEC-3                                                   SIM07260
C                                                                     SIM07270
  390 CONTINUE                                                        SIM07280
C..................................................                   SIM07290
C INPUT 'S' MOLECULES                                                 SIM07300
      DO 460 J=1,NAD                                                  SIM07310
      IF(KR.LT.2)GO TO 460                                            SIM07320
      ANEW1=FNN1(1,J,KR-1)                                            SIM07330
      IF(ANEW1.LE..00001)GO TO 420                                    SIM07340
      NEW1=ANEW1                                                      SIM07350
      REM=ANEW1-NEW1                                                  SIM07360
      CALL RANDU(P)                                                   SIM07370
      IF(P.LT.REM)NEW1=NEW1+1                                         SIM07380
      DO 402 I1=1,NEW1                                                SIM07390
      CALL RANDU(P)                                                   SIM07400
      T=TMIN+DDALFA*(P+FLOAT(J-1))                                    SIM07410
      CALL RANDU(P)                                                   SIM07420
      RNEW=RMIN+P*DR                                                  SIM07430
      CALL RANDU(P)                                                   SIM07440
      TEM=FNN1(4,J,KR-1)                                              SIM07450
      VTER1=SQRT(2.*BOLTZ*TEM/SPEC(1,1))                              SIM07460
      B=VTER1*SQRT(-ALOG(P))                                          SIM07470
      CALL RANDU(P)                                                   SIM07480
      BB=2.*PI*P                                                      SIM07490
      VELX=FNN1(2,J,KR-1)+B*COS(BB)                                   SIM07500
      VELY=FNN1(3,J,KR-1)+B*SIN(BB)                                   SIM07510
      CALL RANDU(P)                                                   SIM07520
      VELZ=VTER1*SQRT(-ALOG(P))                                       SIM07530
C FIND A NEW MOLECULE TO BE ACTIVATED                                 SIM07540
      DO 404 IACT=1,NMOL1                                             SIM07550
      IF(P1(4,IACT).EQ.-99.)GO TO 406                                 SIM07560
  404 CONTINUE                                                        SIM07570
      IF(IACT.EQ.NMOL1)GO TO 3004                                     SIM07580
  406 P1(4,IACT)=RNEW                                                 SIM07590
      P1(5,IACT)=T                                                    SIM07600
      P1(1,IACT)=VELX                                                 SIM07610
      P1(2,IACT)=VELY                                                 SIM07620
  402 P1(3,IACT)=VELZ                                                 SIM07630
  420 CONTINUE                                                        SIM07640
C REPEAT FOR SPECIES 2                                                SIM07650
      ANEW2=FNN2(1,J,KR-1)                                            SIM07660
      IF(ANEW2.LT..00001)GO TO 440                                    SIM07670
      NEW2=ANEW2                                                      SIM07680
      REM=ANEW2-NEW2                                                  SIM07690
      CALL RANDU(P)                                                   SIM07700
      IF(P.LT.REM)NEW2=NEW2+1                                         SIM07710
      DO 422 I2=1,NEW2                                                SIM07720
      CALL RANDU(P)                                                   SIM07730
      T=TMIN+DDALFA*(P+FLOAT(J-1))                                    SIM07740
      CALL RANDU(P)                                                   SIM07750
      RNEW=RMIN+P*DR                                                  SIM07760
      CALL RANDU(P)                                                   SIM07770
      TEM=FNN2(4,J,KR-1)                                              SIM07780
      VTER2=SQRT(2.*BOLTZ*TEM/SPEC(2,1))                              SIM07790
      B=VTER2*SQRT(-ALOG(P))                                          SIM07800
      CALL RANDU(P)                                                   SIM07810
      BB=2.*PI*P                                                      SIM07820
      VELX=FNN2(2,J,KR-1)+B*COS(BB)                                   SIM07830
      VELY=FNN2(3,J,KR-1)+B*SIN(BB)                                   SIM07840
      CALL RANDU(P)                                                   SIM07850
      VELZ=VTER2*SQRT(-ALOG(P))                                       SIM07860
C FIND A NEW MOLECULE TO BE ACTIVATED                                 SIM07870
      DO 424 IACT=1,NMOL2                                             SIM07880
      IF(P2(4,IACT).EQ.-99)GO TO 426                                  SIM07890
  424 CONTINUE                                                        SIM07900
      IF(IACT.EQ.NMOL2)GO TO 3004                                     SIM07910
  426 P2(4,IACT)=RNEW                                                 SIM07920
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```
      P2(5,IACT)=T                                                    SIM07930
      P2(1,IACT)=VELX                                                 SIM07940
      P2(2,IACT)=VELY                                                 SIM07950
  422 P2(3,IACT)=VELZ                                                 SIM07960
  440 CONTINUE                                                        SIM07970
C.....................................................................SIM07980
C REPEAT FOR SPEC-3                                                   SIM07990
C..................................................................... SIM08000
C INPUT 'N' MOLECULES.................................................SIM08010
C SPEC-1                                                              SIM08020
      ANEW1=FSN1(1,J,KR+1)                                            SIM08030
      IF(ANEW1.LE..00001)GO TO 450                                    SIM08040
      NEW1=ANEW1                                                      SIM08050
      REM=ANEW1-NEW1                                                  SIM08060
      CALL RANDU(P)                                                   SIM08070
      IF (P.LT.REM)NEW1=NEW1+1                                        SIM08080
      DO 442 I1=1,NEW1                                                SIM08090
      CALL RANDU(P)                                                   SIM08100
      T=TMIN +DDALFA*(P+FLOAT(J-1))                                   SIM08110
      CALL RANDU(P)                                                   SIM08120
      RNEW=RMAX-P*DR                                                  SIM08130
      CALL RANDU(P)                                                   SIM08140
      TEM=FSN1(4,J,KR+1)                                              SIM08150
      VTER1=SQRT(2.*BOLTZ*TEM/SPEC(1,1))                              SIM08160
      B=VTER1*SQRT(-ALOG(P))                                          SIM08170
      CALL RANDU(P)                                                   SIM08180
      BB=2.*PI*P                                                      SIM08190
      VELX=FSN1(2,J,KR+1)+B*COS(BB)                                   SIM08200
      VELY=FSN1(3,J,KR+1)+B*SIN(BB)                                   SIM08210
      CALL RANDU(P)                                                   SIM08220
      VELZ=VTER1*SQRT(-ALOG(P))                                       SIM08230
C FIND A NEW MOLECULE TO BE ACTIVATED                                 SIM08240
      DO 444 IACT=1,NMOL1                                             SIM08250
      IF(P1(4,IACT).EQ.-99.)GO TO 446                                 SIM08260
  444 CONTINUE                                                        SIM08270
      IF(IACT.EQ.NMOL1)GO TO 3004                                     SIM08280
  446 P1(4,IACT)=RNEW                                                 SIM08290
      P1(5,IACT)=T                                                    SIM08300
      P1(1,IACT)=VELX                                                 SIM08310
      P1(2,IACT)=VELY                                                 SIM08320
  442 P1(3,IACT)=VELZ                                                 SIM08330
  450 CONTINUE                                                        SIM08340
C..................................................................... SIM08350
C INPUT N MOLECULES SPEC-2                                            SIM08360
      ANEW2=FSN2(1,J,KR+1)                                            SIM08370
      IF(ANEW2.LE..00001)GO TO 460                                    SIM08380
      NEW2=ANEW2                                                      SIM08390
      REM=ANEW2-NEW2                                                  SIM08400
      CALL RANDU(P)                                                   SIM08410
      IF(P.LT.REM)NEW2=NEW2+1                                         SIM08420
      DO 452 I2=1,NEW2                                                SIM08430
      CALL RANDU(P)                                                   SIM08440
      T=TMIN+DDALFA*(P+FLOAT(J-1))                                    SIM08450
      CALL RANDU(P)                                                   SIM08460
      RNEW=RMAX-P*DR                                                  SIM08470
      CALL RANDU(P)                                                   SIM08480
      TEM=FSN2(4,J,KR+1)                                              SIM08490
      VTER2=SQRT(2.*BOLTZ*TEM/SPEC(2,1))                              SIM08500
      B=VTER2*SQRT(-ALOG(P))                                          SIM08510
      CALL RANDU(P)                                                   SIM08520
      BB=2*PI*P                                                       SIM08530
      VELX=FSN2(2,J,KR+1)+B*COS(BB)                                   SIM08540
      VELY=FSN2(3,J,KR+1)+B*SIN(BB)                                   SIM08550
      CALL RANDU(P)                                                   SIM08560
      VELZ=VTER2*SQRT(-ALOG(P))                                       SIM08570
C FIND A NEW MOLECULE TO BE ACTIVATED                                 SIM08580
      DO 454 IACT=1,NMOL2                                             SIM08590
      IF(P2(4,IACT).EQ.-99)GO TO 456                                  SIM08600
  454 CONTINUE                                                        SIM08610
      IF(IACT.EQ.NMOL2)GO TO 3004                                     SIM08620
  456 P2(4,IACT)=RNEW                                                 SIM08630
      P2(5,IACT)=T                                                    SIM08640
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      P2(1,IACT)=VELX                                                   SIM086
      P2(2,IACT)=VELY                                                   SIM086
  452 P2(3,IACT)=VELZ                                                   SIM086
  460 CONTINUE                                                          SIM086
C                                                                       SIM086
C                                                                       SIM087
C*****************************************************************************SIM087
C*****************************************************************************SIM087
C REARRANGE MOLECULES IN THEIR CELLS                                    SIM087
C INITIALIZATION                                                        SIM087
 5000 CONTINUE                                                          SIM087
C*************************************************************          SIM087
      KIP=NMOL1+NMOL2+NMOL3                                             SIM087
      DO 1001 KADD=1,KIP                                                SIM087
 1001 IP(KADD)=0                                                        SIM087
      KADD=0                                                            SIM088
      N1A=0                                                             SIM088
      N2A=0                                                             SIM088
      N3A=0                                                             SIM088
C N1A,N2A,N3A ARE THE NUMBER OF ACTIVE MOLECULES (COUNTED NEXT)         SIM088
C                                                                       SIM088
      DO 1100 I=1,NRD                                                   SIM088
      DO 1100 J=1,NAD                                                   SIM088
C                                                                       SIM088
      DO 1005 K=1,4                                                     SIM088
 1005 IC(K,I,J)=0                                                       SIM089
C                                                                       SIM089
C SET SPECIES 1                                                         SIM089
      N1C=0                                                             SIM089
      N2C=0                                                             SIM089
      N3C=0                                                             SIM089
      NTC=0                                                             SIM089
      DO 1020 K1=1,NMOL1                                                SIM089
      IF(P1(4,K1).EQ.-99.)GO TO 1020                                    SIM089
      RLOC=ABS(C(19,I,J)-P1(4,K1))                                      SIM089
      TLOC=ABS(C(20,I,J)-P1(5,K1))                                      SIM090
      IF(RLOC.GT.DR*.5)GO TO 1020                                       SIM090
      IF(TLOC.GT.DDALFA*.5)GO TO 1020                                   SIM090
C                                                                       SIM090
      N1C=N1C+1                                                         SIM090
      NTC=NTC+1                                                         SIM090
      N1A=N1A+1                                                         SIM090
      IF(NTC.EQ.1)IC(4,I,J)=KADD                                        SIM090
      IC(1,I,J)=IC(1,I,J)+1                                             SIM090
      KADD=KADD+1                                                       SIM090
      IP(KADD)=K1                                                       SIM091
 1020 CONTINUE                                                          SIM091
C SET SPEC-2 MOLECULES.....................................             SIM091
      DO 1040 K2=1,NMOL2                                                SIM091
      IF(P2(4,K2).EQ.-99.)GO TO 1040                                    SIM091
      RLOC=ABS(C(19,I,J)-P2(4,K2))                                      SIM091
      TLOC=ABS(C(20,I,J)-P2(5,K2))                                      SIM091
      IF(RLOC.GT.DR*.5)GO TO 1040                                       SIM091
      IF(TLOC.GT.DDALFA*.5)GO TO 1040                                   SIM091
C                                                                       SIM091
      N2A=N2A+1                                                         SIM092
      NTC=NTC+1                                                         SIM092
      IF(NTC.EQ.1)IC(4,I,J)=KADD                                        SIM092
      IC(2,I,J)=IC(2,I,J)+1                                             SIM092
      KADD=KADD+1                                                       SIM092
      IP(KADD)=K2                                                       SIM092
 1040 CONTINUE                                                          SIM092
 1100 CONTINUE                                                          SIM092
      WRITE(6,1021)N1A,N2A                                              SIM092
 1021 FORMAT('  NUMBER OF ACTIVE MOLECULES SPEC1= ',I5,'  SPEC2=',I5/)  SIM092
C                                                                       SIM093
C                                                                       SIM093
C*****************************************************************************SIM093
C CALCULATE COLLISIONS.....................................BLOCK       SIM093
C EXTERNAL LOOPS ARE OVER CELLS I,J                                     SIM093
C*************************************************************          SIM093
C                                                                       SIM093
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      DO 999 I=1,NRD                                                    SIM09370
      DO 999 J=1,NAD                                                    SIM09380
  999 NCOL(I,J)=0                                                       SIM09390
C                                                                       SIM09400
      DO 900 I=1,NRD                                                    SIM09410
      DO 900 J=1,NAD                                                    SIM09420
C                                                                       SIM09430
      NM(1)=IC(1,I,J)                                                   SIM09440
      NM(2)=IC(2,I,J)                                                   SIM09450
      NM(3)=IC(3,I,J)                                                   SIM09460
      NTOT=NM(1)+NM(2)+NM(3)                                            SIM09470
      DO 900 L=1,3                                                      SIM09480
      DO 900 M=1,3                                                      SIM09490
C NUMBER OF SPECIES IN THE PROGRAM IS 2 (3)                             SIM09500
      KV=(L-1)*3+M                                                      SIM09510
      KT=KV+9                                                           SIM09520
C KV,KT ARE THE ADDRESSES OF RELATIVE VELOCITY AND COLLISION TIMERS     SIM09530
  920 IF(C(KT,I,J).GE.TIME) GO TO 900                                   SIM09540
C C(KT,I,J)IS THE INTEGRATED TIME FOR L-M COLLISION                     SIM09550
      KSEL=0                                                            SIM09560
      KREJ=0                                                            SIM09570
      IF(NM(L).GT.1.AND.NM(M).GT.1)GO TO 912                            SIM09580
C NO COLLISIONS ARE CALCULATED IF THERE ARE NO MOLECULES                SIM09590
  911 C(KT,I,J)=C(KT,I,J)+DTM                                           SIM09600
      GO TO 900                                                         SIM09610
C SELECT NOW THE MOLECULES FOR COLLISION                                SIM09620
  912 IF (KSEL.GE.100)GO TO 911                                         SIM09630
      CALL RANDU(P)                                                     SIM09640
      MOL1=P*NM(L)+.999999                                              SIM09650
      IF(MOL1.EQ.0)MOL1=1                                               SIM09660
C                                                                       SIM09670
      CALL RANDU(P)                                                     SIM09680
      MOL2=P*NM(M)+.999999                                              SIM09690
      IF(MOL2.EQ.0)MOL2=1                                               SIM09700
C                                                                       SIM09710
      KSEL=KSEL+1                                                       SIM09720
C                                                                       SIM09730
C CHECK IF THE SAME MOLECULE HAS BEEN SELECTED TWICE                    SIM09740
      IF(L.EQ.M.AND.MOL1.EQ.MOL2)GO TO 912                              SIM09750
C.....                                                                  SIM09760
C FIND THE ACTUAL ADDRESSES OF THE SELECTED MOLECULES                   SIM09770
      IF(L.EQ.1)K1=0                                                    SIM09780
      IF(L.EQ.2)K1=NM(1)                                                SIM09790
      IF(L.EQ.3)K1=NM(1)+NM(2)                                          SIM09800
      IF(M.EQ.1)K2=0                                                    SIM09810
      IF(M.EQ.2)K2=NM(1)                                                SIM09820
      IF(M.EQ.3)K2=NM(1)+NM(2)                                          SIM09830
      KAD1=MOL1+K1+IC(4,I,J)                                            SIM09840
      KAD2=MOL2+K2+IC(4,I,J)                                            SIM09850
C KAD1,KAD2 ARE THE LOCATION OF SELECTED MOLECULES IN IP(  )            SIM09860
      MAD1=IP(KAD1)                                                     SIM09870
      MAD2=IP(KAD2)                                                     SIM09880
C MAD1,MAD2 ARE THE ACTUAL ADDRESSES OF THE SELECTED MOLECULES (THE     SIM09890
C INDICATION OF WHAT SPECIES THEY ARE HAS BEEN DEFINED HERE)            SIM09900
      DO 930 N=1,3                                                      SIM09910
      IF(L.EQ.1)VN1=P1(N,MAD1)                                          SIM09920
      IF(L.EQ.2)VN1=P2(N,MAD1)                                          SIM09930
C     IF(L.EQ.3)VN1=P3(N,MAD1)                                          SIM09940
C                                                                       SIM09950
      IF(M.EQ.1)VN2=P1(N,MAD2)                                          SIM09960
      IF(M.EQ.2)VN2=P2(N,MAD2)                                          SIM09970
C     IF(M.EQ.3)VN2=P3(N,MAD2)                                          SIM09980
C                                                                       SIM09990
  930 VRC(N)=VN1-VN2                                                    SIM10000
C VRC(3) CONTAIN THE THREE RELATIVE VELOCITY COMPONENTS                 SIM10010
      VR=SQRT(VRC(1)*VRC(1)+VRC(2)*VRC(2)+VRC(3)*VRC(3))                SIM10020
C VR IS THE RELATIVE SPEED IN A SPECIFIC COLLISION                      SIM10030
      IF(C(KV,I,J).LT.VR)C(KV,I,J)=VR                                   SIM10040
C LAST STATEMENT RESETS THE MAXIMUM RELATIVE VELOCITY FOR FURTHER        SIM10050
C CALCULATIONS                                                          SIM10060
C                                                                       SIM10070
      IF(KREJ.GT.100)GO TO 911                                          SIM10080
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C                                                                       SIM1009
      CALL RANDU(P)                                                     SIM1010
      AVR=VR/C(KV,I,J)                                                  SIM1011
      KREJ=KREJ+1                                                       SIM1012
      IF(AVR.LT.P)GO TO 912                                             SIM1013
C LAST STATEMENT REJECTS THE CALCULATED COLLISION                       SIM1014
C                                                                       SIM1015
C NOW A SPECIES L-M COLLISION HAS BEEN SELECTED                         SIM1016
C                                                                       SIM1017
C CALCULATE NOW THE PROBABILITY THAT SUCH A COLLISION WILL BE COUNTED   SIM1018
C FOR THE L AND M SPECIES RESPECTIVELY                                  SIM1019
      LP=1                                                              SIM1020
      LM=1                                                              SIM1021
      CALL RANDU(P)                                                     SIM1022
      ANM=FLOAT(NM(L))/FLOAT(NM(M))                                     SIM1023
      IF(ANM.GT.1.)GO TO 950                                            SIM1024
      IF(ANM.LT.P)MP=0                                                  SIM1025
      GO TO 955                                                         SIM1026
C                                                                       SIM1027
C                                                                       SIM1028
  950 ANM=1./ANM                                                        SIM1029
      IF(ANM.LT.P)LP=0                                                  SIM1030
C                                                                       SIM1031
C                                                                       SIM1032
  955 CXS=PI*(SPEC(L,2)+SPEC(M,2))**2/4.                                SIM1033
      ALP=LP                                                            SIM1034
      ALM=LM                                                            SIM1035
C                                                                       SIM1036
      VOLUME=REG(4,KR,KS)*VOL(I)                                        SIM1037
C.....................................................CHECK              SIM1038
      DNL=FLOAT(NM(L))/VOLUME                                           SIM1039
      DNM=FLOAT(NM(M))/VOLUME                                           SIM1040
C USE EQ.10.3                                                           SIM1041
      TOC(L,M)=ALP/(CXS*DNM*VR*NM(L))+ALM/(CXS*DNL*VR*NM(M))            SIM1042
C                                                                       SIM1043
C SET THIS VALUE INTO C(KT,I,J)                                         SIM1044
      C(KT,I,J)=C(KT,I,J)+TOC(L,M)                                      SIM1045
C.................................................                      SIM1046
C SAMPLE THIS COLLISION                                                 SIM1047
      NCOL(I,J)=NCOL(I,J)+1                                             SIM1048
C                                                                       SIM1049
C FIND RELATIVE MASSES                                                  SIM1050
      CALL RANDU(P)                                                     SIM1051
      BB=1.-2.*P                                                        SIM1052
      AA=SQRT(1.-BB*BB)                                                 SIM1053
      VRC(1)=BB*VR                                                      SIM1054
      CALL RANDU(P)                                                     SIM1055
      BB=2.*PI*P                                                        SIM1056
      VRC(2)=AA*COS(BB)*VR                                              SIM1057
      VRC(3)=AA*SIN(BB)*VR                                              SIM1058
C                                                                       SIM1059
C FIND RELATIVE MASSES                                                  SIM1060
      SM=SPEC(L,1)+SPEC(M,1)                                            SIM1061
      RML=SPEC(L,1)/SM                                                  SIM1062
      RMM=SPEC(M,1)/SM                                                  SIM1063
C                                                                       SIM1064
C***********************************************************************SIM1065
C CALCULATE HERE THE ACTUAL ADDRESSES OF COLLIDING MOLECULES AND SET    SIM1066
C THEIR NEW VELOCITIES (NEW VELOCITY COMPONENTS ARE ADDED TO THE        SIM1067
C VELOCITY OF THE CENTER OF MASS VCCM)                                  SIM1068
      DO 960 N=1,3                                                      SIM1069
      IF(L.EQ.1)V1=P1(N,MAD1)                                           SIM1070
      IF(L.EQ.2)V1=P2(N,MAD1)                                           SIM1071
C     IF(L.EQ.3)V1=P3(N,MAD1)                                           SIM1072
      IF(M.EQ.1)V2=P1(N,MAD2)                                           SIM1073
      IF(M.EQ.2)V2=P2(N,MAD2)                                           SIM1074
C     IF(M.EQ.3)V2=P3(N,MAD2)                                           SIM1075
C                                                                       SIM1076
      VCCM=RML*V1+RMM*V2                                                SIM1077
      VCCM1=VCCM+VRC(N)*RMM                                             SIM1078
      VCCM2=VCCM-VRC(N)*RML                                             SIM1079
C                                                                       SIM1080
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C CHANGE IN VELOCITY IS INPUTED ONLY IF PROBABILITY OF COLLISION.GT.1   SIM10810
      IF(LP.NE.1)GO TO 961                                              SIM10820
      IF(L.EQ.1)P1(N,MAD1)=VCCM1                                        SIM10830
      IF(L.EQ.2)P2(N,MAD1)=VCCM1                                        SIM10840
C     IF(L.EQ.3)P3(N,MAD1)=VCCM1                                        SIM10850
C                                                                       SIM10860
  961 IF(LM.NE.1)GO TO 960                                              SIM10870
      IF(M.EQ.1)P1(N,MAD2)=VCCM2                                        SIM10880
      IF(M.EQ.2)P2(N,MAD2)=VCCM2                                        SIM10890
C     IF(M.EQ.3)P3(N,MAD2)=VCCM2                                        SIM10900
C                                                                       SIM10910
  960 CONTINUE                                                          SIM10920
      GO TO 920                                                         SIM10930
  900 CONTINUE                                                          SIM10940
      WRITE(6,4545)TOC(1,1),TOC(1,2),TOC(2,1),TOC(2,2),TIME             SIM10950
 4545 FORMAT(' TIME',5E10.3)                                            SIM10960
C                                                                       SIM10970
C*******************END OF COLLISIONS*************************************SIM10980
C NOW NEW TEMPERATURES MAY BE CALCULATED IN EACH CELL                   SIM10990
C AVERAGE VELOCITY IN CELLS                                             SIM11000
C                                                                       SIM11010
      WRITE(6,4547)                                                     SIM11020
 4547 FORMAT('0    I    J  N1E   N2E     TEMPR1      TEMPR2       VAVX1 SIM11030
     1   VAVY1       VAVX2       VAVY2       NCOL',/)                   SIM11040
C                                                                       SIM11050
      DO 1110 I=1,NRD                                                   SIM11060
      DO 1110 J=1,NAD                                                   SIM11070
      N1E=IC(1,I,J)                                                     SIM11080
      N2E=IC(2,I,J)                                                     SIM11090
      KAD1=IC(4,I,J)                                                    SIM11100
      KAD2=IC(4,I,J)+N1E                                                SIM11110
      IF(N1E.LT.1)GO TO 1112                                            SIM11120
C                                                                       SIM11130
      VX1=0.                                                            SIM11140
      VX2=0.                                                            SIM11150
      VY1=0.                                                            SIM11160
      VY2=0.                                                            SIM11170
C                                                                       SIM11180
      DO 1111 IM=1,N1E                                                  SIM11190
      MAD1=KAD1+IM                                                      SIM11200
      IAD=IP(MAD1)                                                      SIM11210
      VX1=VX1+P1(1,IAD)                                                 SIM11220
 1111 VY1=VY1+P1(2,IAD)                                                 SIM11230
 1112 IF(N2E.LE.0)GO TO 1110                                            SIM11240
C                                                                       SIM11250
      DO 1115 IM=1,N2E                                                  SIM11260
      MAD2=MAD1+IM                                                      SIM11270
      IAD=IP(MAD2)                                                      SIM11280
      VX2=VX2+P2(1,IAD)                                                 SIM11290
 1115 VY2=VY2+P2(2,IAD)                                                 SIM11300
C                                                                       SIM11310
C THE AVERAGE VELOCITIES IN THE CELL WILL RESULT-                       SIM11320
      VAVX1=VX1/N1E                                                     SIM11330
      VAVY1=VY1/N1E                                                     SIM11340
      VAVX2=VX2/N2E                                                     SIM11350
      VAVY2=VY2/N2E                                                     SIM11360
      IF(I.NE.1)GO TO 1116                                              SIM11370
C                                                                       SIM11380
      FSN1(2,J,KR)=VAVX1+FSN1(2,J,KR)                                   SIM11390
      FSN1(3,J,KR)=VAVY1+FSN1(3,J,KR)                                   SIM11400
      FSN2(2,J,KR)=VAVX2+FSN2(2,J,KR)                                   SIM11410
      FSN2(3,J,KR)=VAVY2+FSN2(3,J,KR)                                   SIM11420
C                                                                       SIM11430
 1116 IF(I.NE.NRD)GO TO 1117                                            SIM11440
      FNN1(2,J,KR)=VAVX1+FNN1(2,J,KR)                                   SIM11450
      FNN1(3,J,KR)=VAVY1+FNN1(3,J,KR)                                   SIM11460
      FNN2(2,J,KR)=VAVX2+FNN2(2,J,KR)                                   SIM11470
      FNN2(3,J,KR)=VAVY2+FNN2(3,J,KR)                                   SIM11480
C                                                                       SIM11490
 1117 IF(J.NE.1)GO TO 1118                                              SIM11500
      FEN1(2,I)=VAVX1+FEN1(2,I)                                         SIM11510
      FEN1(3,I)=VAVY1+FEN1(3,I)                                         SIM11520
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      FEN2(2,I)=VAVX2+FEN2(2,I)                                          SIM11530
      FEN2(3,I)=VAVY2+FEN2(3,I)                                          SIM11540
C                                                                        SIM11550
 1118 IF(J.NE.NAD)GO TO 1119                                             SIM11560
      FWN1(2,I)=VAVX1+FWN1(2,I)                                          SIM11570
      FWN1(3,I)=VAVY1+FWN1(3,I)                                          SIM11580
      FWN2(2,I)=VAVX2+FWN2(2,I)                                          SIM11590
      FWN2(3,I)=VAVY2+FWN2(3,I)                                          SIM11600
 1119 CONTINUE                                                           SIM11610
C                                                                        SIM11620
C THERMAL VELOCITIES AND TEMPERATURES                                    SIM11630
      ENRG1=0.                                                           SIM11640
      ENRG2=0.                                                           SIM11650
      IF(N1E.LT.1)GO TO1131                                              SIM11660
      DO 1130 IM=1,N1E                                                   SIM11670
      MAD1=KAD1+IM                                                       SIM11680
      IAD=IP(MAD1)                                                       SIM11690
      CX1=P1(1,IAD)-VAVX1                                                SIM11700
      CY1=P1(2,IAD)-VAVY1                                                SIM11710
      CZ1=P1(3,IAD)                                                      SIM11720
 1130 ENRG1=ENRG1+CX1*CX1+CY1*CY1+CZ1*CZ1                                SIM11730
 1131 IF(N2E.LT.1)GO TO 1150                                             SIM11740
      DO 1140 IM=1,N2E                                                   SIM11750
      MAD2=KAD2+IM                                                       SIM11760
      IAD=IP(MAD2)                                                       SIM11770
      CX2=P2(1,IAD)-VAVX2                                                SIM11780
      CY2=P2(2,IAD)-VAVY2                                                SIM11790
      CZ2=P2(3,IAD)                                                      SIM11800
C                                                                        SIM11810
C                                                                        SIM11820
 1140 ENRG2=ENRG2+CX2*CX2+CY2*CY2+CZ2*CZ2                                SIM11830
C                                                                        SIM11840
 1150 TEMPR1=(ENRG1/N1E)*SPEC(1,1)/(3.*BOLTZ)                            SIM11850
      TEMPR2=(ENRG2/N2E)*SPEC(2,1)/(3.*BOLTZ)                            SIM11860
C                                                                        SIM11870
      IF(I.NE.1)GO TO 1151                                               SIM11880
      FSN1(4,J,KR)=TEMPR1+FSN1(4,J,KR)                                   SIM11890
      FSN2(4,J,KR)=TEMPR2+FSN2(4,J,KR)                                   SIM11900
C                                                                        SIM11910
 1151 IF(I.NE.NRD)GO TO 1152                                             SIM11920
      FNN1(4,J,KR)=TEMPR1+FNN1(4,J,KR)                                   SIM11930
      FNN2(4,J,KR)=TEMPR2+FNN2(4,J,KR)                                   SIM11940
C                                                                        SIM11950
 1152 IF(J.NE.1)GO TO 1153                                               SIM11960
      FWN1(4,I)=TEMPR1+FWN1(4,I)                                         SIM11970
      FWN2(4,I)=TEMPR2+FWN2(4,I)                                         SIM11980
C                                                                        SIM11990
 1153 IF(J.NE.NAD)GO TO 1154                                             SIM12000
      FEN1(4,I)=TEMPR1+FEN1(4,I)                                         SIM12010
      FEN2(4,I)=TEMPR2+FEN2(4,I)                                         SIM12020
 1154 CONTINUE                                                           SIM12030
C                                                                        SIM12040
      WRITE(6,4548)I,J,N1E,N2E,TEMPR1,TEMPR2,VAVX1,VAVY1,VAVX2,VAVY2,NCOSIM12050
     1L(I,J)                                                             SIM12060
 4548 FORMAT(' ',4I5,6F12.3,I7)                                          SIM12070
C                                                                        SIM12080
 1110 CONTINUE                                                           SIM12090
C                                                                        SIM12100
 6000 CONTINUE                                                           SIM12110
C CALCULATE AVERAGED PARAMETERS, WEIGHTED BY DFI                         SIM12120
      DO 6010 I=1,NRD                                                    SIM12130
      DO 6010 KPAR=1,4                                                   SIM12140
      FOW1(KPAR,I,KR,KS)=FWN1(KPAR,I)/(NIS)                              SIM12150
      FOW2(KPAR,I,KR,KS)=FWN2(KPAR,I)/(NIS)                              SIM12160
      FOE1(KPAR,I,KR,KS)=FEN1(KPAR,I)/(NIS)                              SIM12170
 6010 FOE2(KPAR,I,KR,KS)=FEN2(KPAR,I)/(NIS)                              SIM12180
C                                                                        SIM12190
      DO 6020 J=1,NAD                                                    SIM12200
      DO 6020 KPAR=1,4                                                   SIM12210
      FSN1(KPAR,J,KR)=FSN1(KPAR,J,KR)/NIS                                SIM12220
      FSN2(KPAR,J,KR)=FSN2(KPAR,J,KR)/NIS                                SIM12230
      FNN1(KPAR,J,KR)=FNN1(KPAR,J,KR)/NIS                                SIM12240
```

```
 6020 FNN2(KPAR,J,KR)=FNN2(KPAR,J,KR)/NIS                                SIM12250
C                                                                        SIM12260
C TO PREPARE FLOWS FOR THE NEXT REGION OR SECTOR, DIVIDE F()N() BY LOCALSIM12270
C DFI AND MULTIPLY BY NEXT DFI WHEN STARTING NEW REGION                  SIM12280
C                                                                        SIM12290
C CALCULATE HERE THE MEAN FREE PATH AND STORE INTO REG(,,)               SIM12300
C                                                                        SIM12310
C STOP PROGRAM IF FLOW BECOMES COLLISIONLESS OR NUMBER DENSITY IS EQUAL SIM12320
C TO THE AMBIENT NUMBER DENSITY. STORE FOE1,FOE2 IN A SEPARATE FILE TO  SIM12330
C BE USED IN A DIFFERENT PROGRAM.                                        SIM12340
C                                                                        SIM12350
C PRINT AVERAGED RESULTS                                                 SIM12360
      WRITE(6,6029)                                                      SIM12370
 6029 FORMAT(' ',////)                                                   SIM12380
      WRITE(6,6030)NIS,KR                                                SIM12390
 6030 FORMAT(' AVERAGED OUTPUT FLOWS AFTER',I5,' TIME INCREMENTS IN REGI SIM12400
     1ON',I5)                                                            SIM12410
      WRITE(6,6031)                                                      SIM12420
 6031 FORMAT('0    I    FEN1(1,I)    FEN2(1,I)    FWN1(1,I)   FWN2(1,I)'SIM12430
     1)                                                                  SIM12440
      DO 6033 I=1,NRD                                                    SIM12450
      WRITE(6,6032)I,FEN1(1,I),FEN2(1,I),FWN1(1,I),FWN2(1,I)             SIM12460
 6032 FORMAT(' ',I5,4F13.3)                                              SIM12470
 6033 CONTINUE                                                           SIM12480
      WRITE (6,6034)                                                     SIM12490
 6034 FORMAT('0    J    FNN1(1,J,KR)   FNN2(1,J,KR)   FSN1(1,J,KR)   FSNSIM12500
     12(1,J,KR)')                                                        SIM12510
      DO 6036 J=1,NAD                                                    SIM12520
      WRITE(6,6037)J,FNN1(1,J,KR),FNN2(1,J,KR),FSN1(1,J,KR),FSN2(1,J,KR)SIM12530
 6037 FORMAT(' ',I5,4F15.5)                                              SIM12540
 6036 CONTINUE                                                           SIM12550
C                                                                        SIM12560
C************************************************************************SIM12570
C                                                                        SIM12580
C START A NEW REGION                                                     SIM12590
C     IF(KR.EQ.10) GO TO 7000                                            SIM12600
C     KR=KR+1                                                            SIM12610
C     GO TO 2000                                                         SIM12620
C                                                                        SIM12630
C************************************************************************SIM12640
C                                                                        SIM12650
 7000 CONTINUE                                                           SIM12660
C                                                                        SIM12670
C                                                                        SIM12680
C************************************************************************SIM12690
C                                                                        SIM12700
C FIND IF FLOW BECAME COLLISIONLESS IN THE WHOLE SECTOR                  SIM12710
C IF POSITIVE, STORE FOE1,FOE2 IN A SEPARATE FILE AND STOP PROGRAM       SIM12720
C                                                                        SIM12730
C PREPARE DATA FOR THE NEXT SECTOR                                       SIM12740
C     KR=1                                                               SIM12750
C     STOP PROGRAM IF KS WAS BOUNDED BY THE WALL                         SIM12760
C     KS=KS+1                                                            SIM12770
C     GO TO 1000                                                         SIM12780
C                                                                        SIM12790
C************************************************************************SIM12800
C                                                                        SIM12810
C IF THERE IS BACK FLOW (FWN1,FWN2) NONZERO CALCULATE NEXT ITERATION     SIM12820
C     ITER=ITER+1                                                        SIM12830
C     KS=KR=1                                                            SIM12840
C     GO TO 3000                                                         SIM12850
C                                                                        SIM12860
C************************************************************************SIM12870
C                                                                        SIM12880
      WRITE(6,6099)                                                      SIM12890
 6099 FORMAT('1 DATA FOR TEN MOLECULES SPEC.2')                          SIM12900
      DO 3003 I=1,10                                                     SIM12910
      WRITE(6,3002) P2(1,I),P2(2,I),P2(3,I),P2(4,I),P2(5,I)              SIM12920
 3002 FORMAT(' ',4F10.3,E18.10)                                          SIM12930
 3003 CONTINUE                                                           SIM12940
      GO TO 3009                                                         SIM12950
 3004 WRITE(6,3005)                                                      SIM12960
```

```
 3005 FORMAT(' NO PLACE FOR ADDITIONAL MOLECULES')                    SIM12970
 3009 CONTINUE                                                        SIM12980
      STOP                                                            SIM12990
      END                                                             SIM13000
C                                                                     SIM13010
C                                                                     SIM13020
      SUBROUTINE RANDU(P)                                             SIM13030
      COMMON IX                                                       SIM13040
      IY = IX*65539                                                   SIM13050
      IF (IY) 5,6,6                                                   SIM13060
    5 IY = IY+2147483647+1                                            SIM13070
    6 P = IY                                                          SIM13080
      P = P*.4656613E-9                                               SIM13090
      IX = IY                                                         SIM13100
      RETURN                                                          SIM13110
      END                                                             SIM13120
```

B.5 Program SIMUL - User's Guide

Preparation: Run AXSYM program. From its output data evaluate:

ALFA - The averaged angle for the continuum breakdown

($P \sim 0.05$)

TETA - Flow direction along the breakdown limit.

Flow parameters along this line - Pressure, temperature, velocity, mean free path.

Input Data:

Radius of nozzle ring	R1
Radial size of a cell	DR
Maximum radius in simulation	RP
Angle of breakdown limit	ALFA
Flow direction along (ALFA)	TETA
Averaged flow velocity along (ALFA)	Vo
Molecular weight of each species	Spec(I,1)
Molecular diameter of each species	Spec (I,2)
Mean free path along (ALFA)	FPM
Averaged Temperature (ALFA)	TEMP
Time increment	DTM
Number of time increments	NIS

Options

a. Geometry

The program is designed to run for axisymmetric ring flow.

For a two dimensional planar flow the molecular motion, collisions and flow calculation remain unchanged. The flow cross section remain

unchanged. Instead of the angle DFI the two dimensional flow requires the definition of the width of each region (or cell). To keep the number of molecules within reasonable computational limits this size has to decrease in the same manner as DFI.

The part of the program which has to be changed for this purpose is lines 230 to 250.

b. Wall flux calculations:

The program may run for the whole molecular region resulting the flux towards the wall (this part needs additional debugging). However in order to make it more efficient we may stop the program at a sector where the flow becomes collisionless. The remaining part of the flow may be regarded either as collisionless or if we define a much larger size of cells we may calculate the molecular collisions on this basis.

This part need additional analysis and programming.

Execution Commands

Without additional changes the program runs under WATFIV compiler using the following command:

```
WATFI AXSYM * (XTYPE)
```

Further developments will be required to run the program for each sector separately and the output intermediate results on the mass storage.

B.6 The Influence of the Ambient Gas

The temperature, pressure and density of the ambient gas are shown in Table 1. Because its temperature is much higher than in the jet gas, the thermal velocity of ambient gas molecules is much higher than jet molecules. the following contribution may be expected due to the ambient gas:

a. Collisions between the "hot" ambient molecules with the "cold" jet molecules may cause an increase in the dissipation in the outer layer of the jet and increase in the flux towards the walls.

b. For higher ambient pressures, those collisions become rare because of the low number density therefore, the influence of the collisions may decrease.

The only way to evaluate the influence of these two controversial factors is by an additional simulation program to be designed for this region. The following are the main factors to be included in this program:

Boundary Conditions:

a. The jet side: FOE1 and FOE2 obtained from the last simulated sector (SIMUL) supply the number flux, flow velocity componetns and temperatures. These parameters are given for all points along the radius R(I) at constant distances DR. In the low density domain the resolution DR is much too large compared with the expected mean free path. A different mesh has to be designed for this purpose. It is possible that one cell may be sufficient.

b. Far Field Condition: The boundary conditions where the gas may be regarded "undisturbed" by the jet are as follows

- Jet gas molecules are allowed to go out the simulation region (these molecules will be regarded as "lost" molecules).
- Ambient gas is allowed to enter the simulated region according with their thermal velocity and number density.

c. Solid Wall Bondaries. The solid wall may be assumed to have a constant temperature T_w. Incident molecules of either species are reflected back from the wall. Different models of collisions with the wall may be employed.

- Elastic collisions 'specular reglection' (this calculation has been included in SIMUL program)
- Collisions with ideal heat transfer (diffuse reflections)
- Other models depending on the materials and surface parameters.

The collision with the wall was included as an internal routine in the program SIMUL. If the general molecular simulation contains the program proposed here the collision with the wall will be omitted from SIMUL and become the core of the additional collisionless program. Figure 25 shows the low density (collisionless) region and its boundaries.

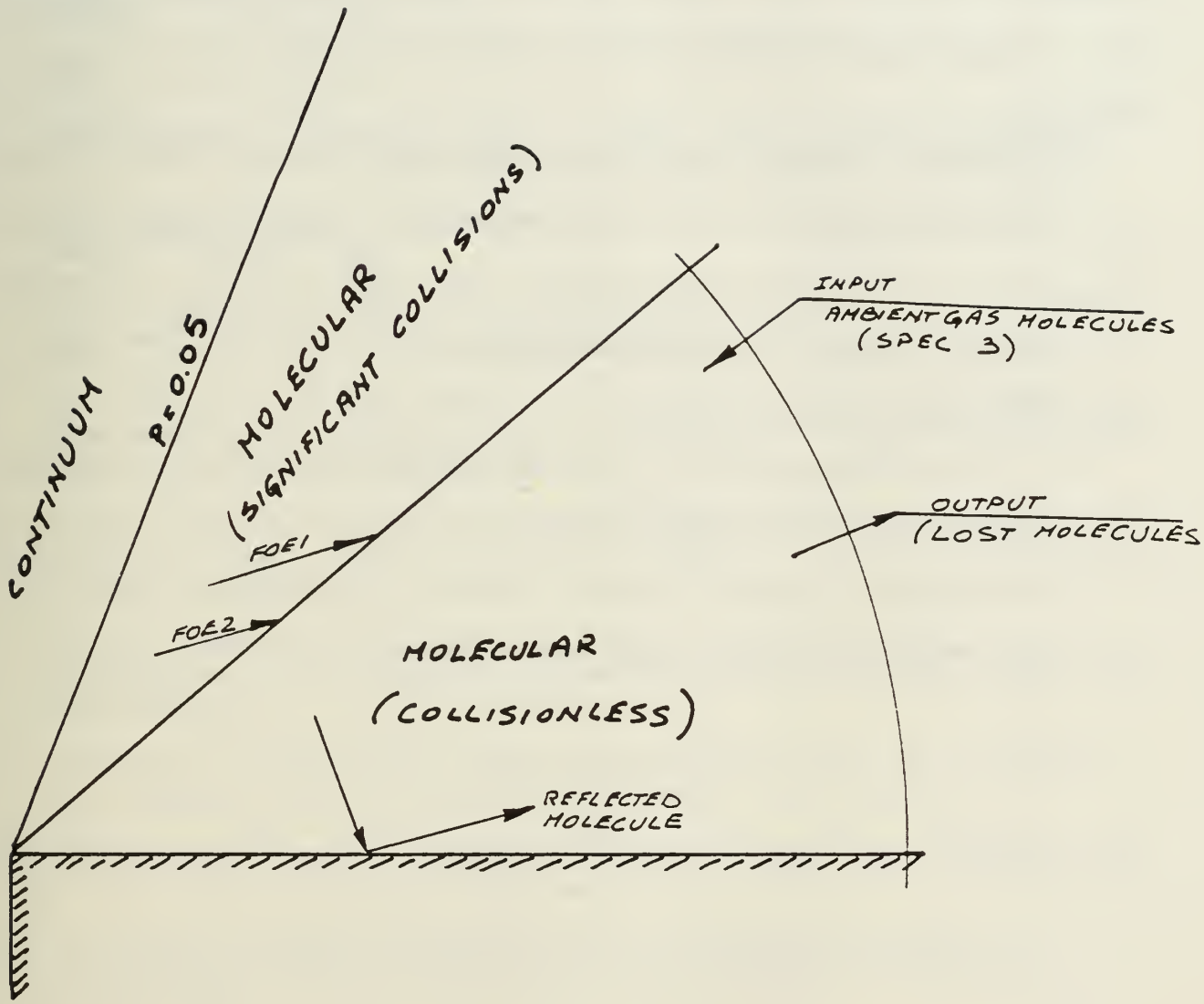

Figure 25. The Low Density Region in the Jet

SUMMARY OF REPORT

Algorithms for the continuum regime and for the region where molecular collisions are significant have been developed.

Program AXSYM contains the calculation of planar jet flow and axisymmetric ring jet flow. This program supplies data for the limits where the continuum approach become invalid and molecular approach should be employed.

Program SIMUL contains the molecular simulation for the axisymmetric ring flow. This program may run for the whole molecular region to result in the calculation of flux towards the solid wall. For a more efficient simulation it is proposed to design an additional program for the collisionless region where ambient gas may be included.

For the two dimensional flow, program SIMUL may be used after changing the definition of the cell geometry.

To run the whole program it may be required to make separate runs for each sector and store results on the mass storage.

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